Access DB# 203221

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: James Galoboy Examiner # : 82785 Date: 9-28-06
Art Unit: 1714 Phone Number 30 Serial Number: 10/783,724
Mail Box and Bldg/Room Location: 10D64 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): _____

_____

Earliest Priority Filing Date: _____

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please see attached.

(NOT MUCH OUT THERE FOR THE CASE WHERE m≠0.)

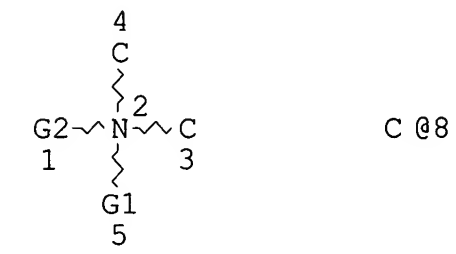
****

STAFF USE ONLY	Type of Search		Vendors and cost where applicable	
Searcher:	Ed	NA Sequence (#)		STN $452.25
Searcher Phone #:		AA Sequence (#)		Dialog
Searcher Location:		Structure (#)	5	Questel/Orbit (substs)
Date Searcher Picked Up:		Bibliographic		Dr.Link
Date Completed:	9-29-06	Litigation		Lexis/Nexis
Searcher Prep & Review Time:	5	Fulltext		Sequence Systems
~~Clerical Prep Time:~~		Patent Family		WWW/Internet
Online Time:	80	Other		Other (specify)

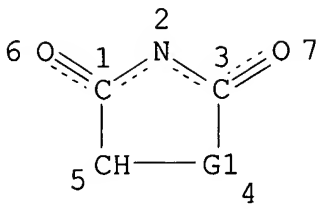
PTO-1590 (8-01)

```
=> FILE REG
FILE 'REGISTRY' ENTERED AT 14:07:47 ON 29 SEP 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 American Chemical Society (ACS)


=> D HIS

     FILE 'LREGISTRY' ENTERED AT 11:39:48 ON 29 SEP 2006
L1                STR
L2                STR
L3                STR L2

     FILE 'REGISTRY' ENTERED AT 11:46:20 ON 29 SEP 2006
L4              2 S L1 AND L3
L5                STR L1
L6             12 S L5 AND L3

     FILE 'HCAPLUS' ENTERED AT 11:50:53 ON 29 SEP 2006
L7            709 S DAHLMAN ?/AU OR DAHLMANN ?/AU
L8            235 S FEUSTEL ?/AU
L9             13 S L7 AND L8
                  SEL L9 1 RN

     FILE 'REGISTRY' ENTERED AT 11:52:57 ON 29 SEP 2006
L10            17 S E1-E17

     FILE 'LREGISTRY' ENTERED AT 11:56:20 ON 29 SEP 2006
L11               STR L5

     FILE 'REGISTRY' ENTERED AT 11:59:52 ON 29 SEP 2006
L12            19 S L11 AND L3
L13               STR
L14            10 S L11 AND L3 NOT L13
L15           156 S L11 AND L3 NOT L13 FUL
                  SAV L15 GOL724/A
L16            61 S L15 AND 4/ELC.SUB
L17            62 S L15 AND 1/NC
L18            55 S L16 AND L17
L19             6 S L16 NOT L18
L20        108024 S C2H4O
L21         57285 S C3H6O
L22             0 S L15 AND (L20 OR L21)
L23             5 S L15 AND L10
L24            12 S L10 NOT L23
L25           101 S L15 NOT L18
                  E C11H21N2O2.CH3O4S/MF
```

```
L26            3 S E3
L27            1 S L26 AND L25
L28           60 S L25 AND (F OR CL OR BR OR I)
L29        10906 S CH3O4S
L30            5 S L25 AND L29
L31           50 S (L28 OR L30) AND 2/NC

     FILE 'HCA' ENTERED AT 14:05:01 ON 29 SEP 2006
                S L13

     FILE 'REGISTRY' ENTERED AT 14:05:03 ON 29 SEP 2006

     FILE 'HCA' ENTERED AT 14:05:04 ON 29 SEP 2006
L32            3 S L18
L33           27 S L31
L34           30 S L32 OR L33

     FILE 'REGISTRY' ENTERED AT 14:07:47 ON 29 SEP 2006


=> D L15 QUE STAT
L3                STR
```



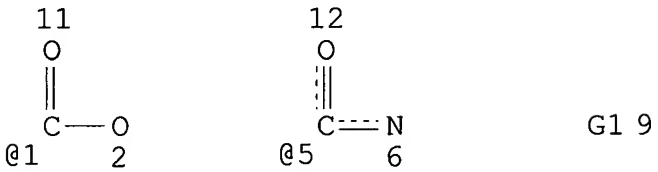

```
VAR G1=8/O
VAR G2=ID/8
NODE ATTRIBUTES:
NSPEC   IS RC     AT   3
NSPEC   IS RC     AT   4
NSPEC   IS RC     AT   8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   6

STEREO ATTRIBUTES: NONE
L11               STR
```



REP G1=(1-5) CH
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
L13 STR



VAR G1=1/5
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
L15 156 SEA FILE=REGISTRY SSS FUL L11 AND L3 NOT L13

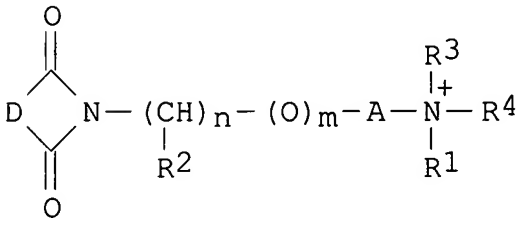
100.0% PROCESSED 32407 ITERATIONS 156 ANSWERS
SEARCH TIME: 00.00.01

=> FILE HCA
FILE 'HCA' ENTERED AT 14:08:21 ON 29 SEP 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

=> D L34 1-30 CBIB ABS HITSTR HITRN

L34 ANSWER 1 OF 30 HCA COPYRIGHT 2006 ACS on STN
141:227837 Corrosion and gas hydrate inhibitors having improved water solubility and increased biodegradability. Dahlmann, Uwe; Feustel, Michael (Clariant GmbH, Germany). U.S. Pat. Appl. Publ. US 2004167040 A1 20040826, 8 pp. (English). CODEN: USXXCO. APPLICATION: US 2004-783724 20040220. PRIORITY: DE 2003-10307725 20030224.

GI



I

AB The compds. of the formula (I) where R1 is C1-22-alkyl, C2-22-alkenyl, C6-30-aryl or C7-30-alkylaryl, -CHR5-COO- or -O-; R2 is hydrogen, -CH3, or -OH, R3, R4 are each independently C1-22-alkyl, C2-22-alkenyl, C6-30-aryl, or C7-30-alkylaryl, R5 is hydrogen, C1-22-alkyl, or C2-22-alkenyl, A is a C2-4-alkylene group, D is a C2-5-alkylene group which may contain one or two heteroatoms, m is a no. from 0 to 30, n is a no. from 1 to 18, are useful as corrosion and gas hydrate inhibitors.

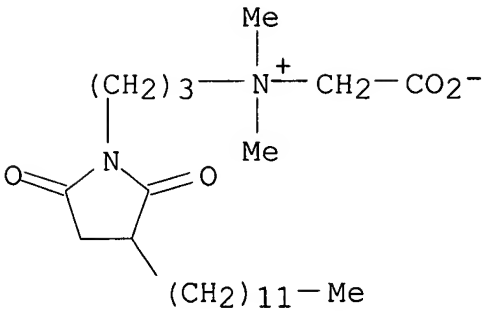
IT **745807-35-6P**
(acorrosion and gas hydrate inhibitors having improved water soly. and increased biodegradability)

RN 745807-35-6 HCA

CN 1-Pyrrolidinepropanaminium, N-(carboxymethyl)-3-(dodecenyl)-N,N-dimethyl-2,5-dioxo-, inner salt (9CI) (CA INDEX NAME)

CM 1

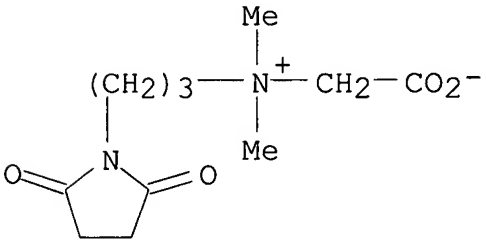
CRN 745807-34-5
CMF C23 H42 N2 O4



IT **745054-51-7DP**, polyisobutenyl derivs. **745807-22-1P** **745807-26-5P** **745807-30-1P**
(corrosion and gas hydrate inhibitors having improved water soly. and increased biodegradability)

RN 745054-51-7 HCA

CN 1-Pyrrolidinepropanaminium, N-(carboxymethyl)-N,N-dimethyl-2,5-dioxo-, inner salt (9CI) (CA INDEX NAME)

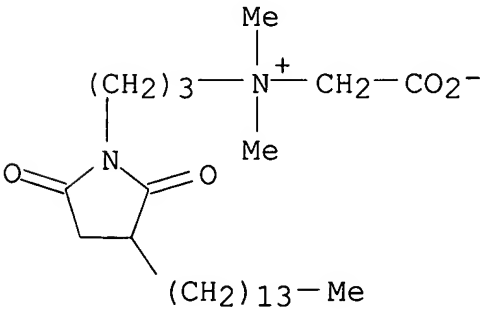


RN 745807-22-1 HCA

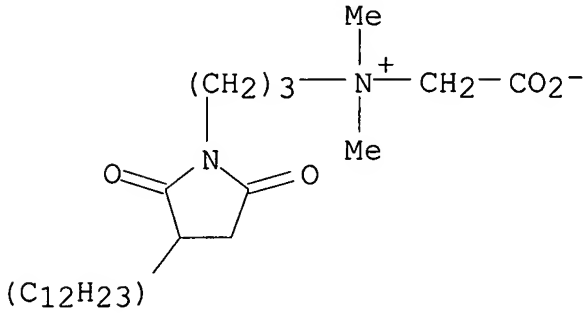
CN 1-Pyrrolidinepropanaminium, N-(carboxymethyl)-N,N-dimethyl-2,5-dioxo-3-(tetradecenyl)-, inner salt (9CI) (CA INDEX NAME)

CM 1

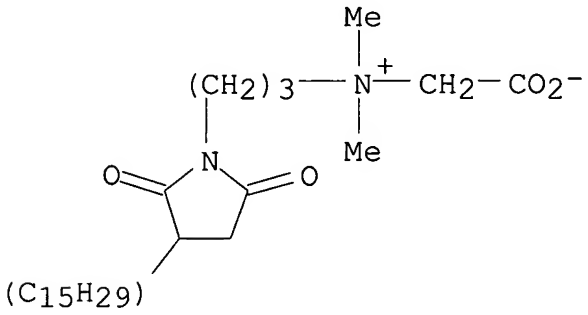
CRN 745807-21-0
CMF C25 H46 N2 O4



RN 745807-26-5 HCA
CN 1-Pyrrolidinepropanaminium, N-(carboxymethyl)-N,N-dimethyl-2,5-dioxo-3-(tetrapropenyl)-, inner salt (9CI) (CA INDEX NAME)



RN 745807-30-1 HCA
CN 1-Pyrrolidinepropanaminium, N-(carboxymethyl)-N,N-dimethyl-2,5-dioxo-3-(pentapropenyl)-, inner salt (9CI) (CA INDEX NAME)



IT **745807-35-6P**
(acorrosion and gas hydrate inhibitors having improved water soly. and increased biodegradability)
IT **745054-51-7DP**, polyisobutenyl derivs. **745807-22-1P** **745807-26-5P** **745807-30-1P**
(corrosion and gas hydrate inhibitors having improved water soly. and increased biodegradability)

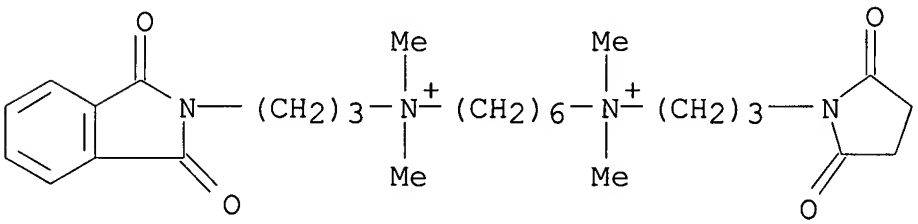
L34 ANSWER 2 OF 30 HCA COPYRIGHT 2006 ACS on STN
141:81700 Development of a New Type of Allosteric Modulator of Muscarinic Receptors: Hybrids of the Antagonist AF-DX 384 and the Hexamethonio Derivative W84. Mohr, Marion; Heller, Eberhard; Ataie, Ameneh; Mohr, Klaus; Holzgrabe, Ulrike (Institute of Pharmacy and Food Chemistry, Pharmaceutical Chemistry, University of Wuerzburg, Wuerzburg, 97074, Germany). Journal of Medicinal Chemistry, 47(12), 3324-3327 (English) 2004. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 141:81700. Publisher: American Chemical Society.

AB Various fragments of the hexamethonio-type allosteric agent W84 were linked to the secondary amino group of the muscarinic M2 acetylcholine receptor-preferring antagonist AF-DX 384 to increase the area of attachment with the allosteric site. Addn. of only the phthalimido moiety of W84 gave an allosteric enhancer of NMS binding. Thus, a new lead structure for the development of allosteric enhancers of NMS binding has been discovered.

IT **269730-39-4P**
(prepn. and muscarinic receptor allosteric modulating activity of AF-DX 384 and hexamethonio deriv. hybrids)

RN 269730-39-4 HCA

CN 1,6-Hexanediaminium, N-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-N'-[3-(2,5-dioxo-1-pyrrolidinyl)propyl]-N,N,N',N'-tetramethyl-, dibromide (9CI) (CA INDEX NAME)



●2 Br^-

IT **269730-39-4P**
(prepn. and muscarinic receptor allosteric modulating activity of AF-DX 384 and hexamethonio deriv. hybrids)

L34 ANSWER 3 OF 30 HCA COPYRIGHT 2006 ACS on STN

140:209903 Contribution of lateral substituents in symmetrical and non-symmetrical heptane-bisammonio compounds to the allosteric stabilization of N-methylscopolamine binding to muscarinic M2 receptors. Staudt, Markus; Traenkle, Christian; Mohr, Klaus; Holzgrabe, Ulrike (Institute of Pharmacy, University of Bonn, Bonn, Germany). Archiv der Pharmazie (Weinheim, Germany), 336(8), 385-389 (English) 2003. CODEN: ARPMAS. ISSN: 0365-6233. Publisher: Wiley-VCH Verlag GmbH & Co. KGaA.

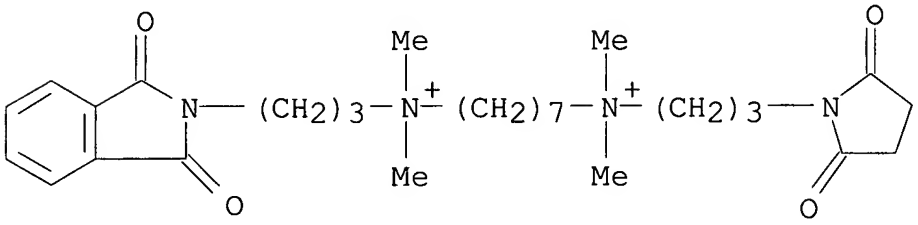
AB Allosteric modulators are able to enhance or decrease the equil. binding of orthosteric agonists or antagonists. The treatment of Alzheimer's disease and the organophosphorus poisoning can take advantage of the enhancement of the ligand binding. Prerequisite is the formation of ternary complexes consisting of the receptor protein, the orthosteric ligand, e.g. N-methylscopolamine (NMS), and the alloster optimized for the corresponding orthoster. In this

study, heptane-bisammonio compds. were optimized with regard to the orthosteric antagonist NMS. Comparing pairs of compds. characterized by phthalimides, cyclohexanedicarbonic acid imide and succinimides at both ends or a phthalimide at one end and either of the three imides at the other end stressed the importance of an arom. moiety at both ends of the heptane-bisammonio chain.

IT **663937-84-6P**
(stabilization of N-methylscopolamine M2 receptors complexes by sym. and non-sym. heptane-bisammonio compds.)

RN 663937-84-6 HCA

CN 1,7-Heptanediaminium, N-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-N'-[3-(2,5-dioxo-1-pyrrolidinyl)propyl]-N,N,N',N'-tetramethyl-, dibromide (9CI) (CA INDEX NAME)

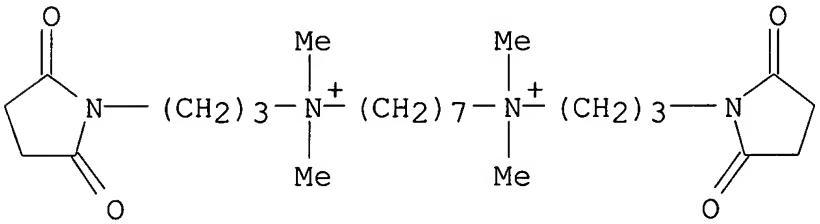


●2 Br^-

IT **202644-30-2P**
(stabilization of N-methylscopolamine M2 receptors complexes by sym. and non-sym. heptane-bisammonio compds.)

RN 202644-30-2 HCA

CN 1,7-Heptanediaminium, N,N'-bis[3-(2,5-dioxo-1-pyrrolidinyl)propyl]-N,N,N',N'-tetramethyl-, dibromide (9CI) (CA INDEX NAME)



●2 Br^-

IT **663937-84-6P**

(stabilization of N-methylscopolamine M2 receptors complexes by sym. and non-sym. heptane-bisammonio compds.)

IT **202644-30-2P**
(stabilization of N-methylscopolamine M2 receptors complexes by sym. and non-sym. heptane-bisammonio compds.)

L34 ANSWER 4 OF 30 HCA COPYRIGHT 2006 ACS on STN

138:331212 Mapping Property Distributions of Molecular Surfaces: Algorithm and Evaluation of a Novel 3D Quantitative Structure-Activity Relationship Technique. Stiefl, Nikolaus; Baumann, Knut (Department of Pharmacy and Food Chemistry, University of Wuerzburg, Wuerzburg, D 97074, Germany). Journal of Medicinal Chemistry, 46(8), 1390-1407 (English) 2003. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.

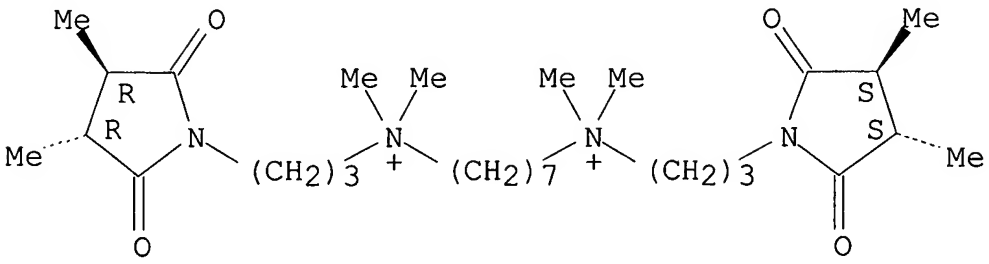
AB A novel mol. descriptor called MaP (mapping property distributions of mol. surfaces) is presented. It combines facile computation, translational and rotational invariance, and straightforward interpretability of the computed models. A three-step procedure is used to compute the MaP descriptor. First, an approxn. to the mol. surface with equally distributed surface points is computed. Next, mol. properties are projected onto this surface. Finally, the distribution of surface properties is encoded into a translationally and rotationally invariant mol. descriptor that is based on radial distribution functions (distance-dependent count statistics). The calcd. descriptor is correlated with biol. data through chemometric regression techniques in combination with a variable selection. The latter is used to identify variables that are highly relevant for the model and hence for its interpretation. Three applications of the new descriptor are presented, each representing a different area of 3D-QSAR. For reasons of comparability, the new descriptor was tested on the steroid "benchmark" data set. Furthermore, a highly diverse data set with potentially eye-irritating compds. was studied, and third, a set of flexible structures with a modulating effect on the muscarinic M2 receptor were studied. Not only were all models highly predictive but interpretation of the back-projected variables into the original mol. space led to biol. and chem. relevant conclusions.

IT **518057-96-0 518057-97-1 518058-02-1 518058-06-5**
(muscarinic M2 receptors modulation by; mapping property distributions of mol. surfaces using algorithm and evaluation of a novel 3D quant. structure-activity relationship technique)

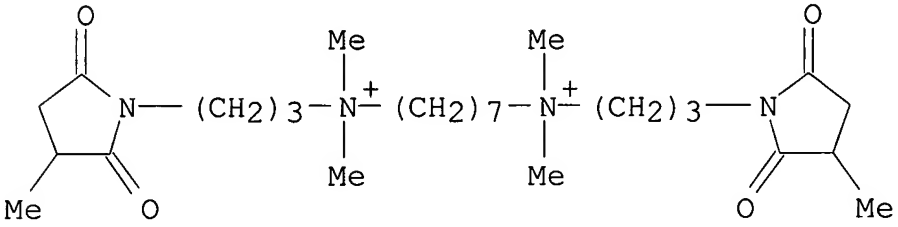
RN 518057-96-0 HCA

CN 1,7-Heptanediaminium, N-[3-[(3R,4R)-3,4-dimethyl-2,5-dioxo-1-pyrrolidinyl]propyl]-N'-[3-[(3S,4S)-3,4-dimethyl-2,5-dioxo-1-pyrrolidinyl]propyl]-N,N,N',N'-tetramethyl-, rel- (9CI) (CA INDEX NAME)

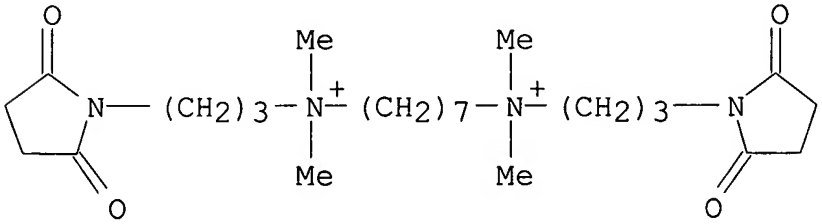
Relative stereochemistry.



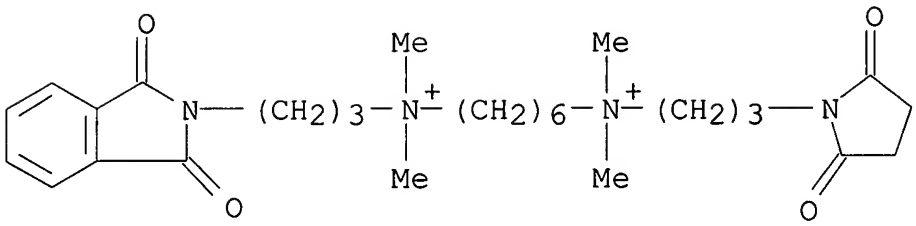
RN 518057-97-1 HCA
CN 1,7-Heptanediaminium, N,N,N',N'-tetramethyl-N,N'-bis[3-(3-methyl-2,5-dioxo-1-pyrrolidinyl)propyl]- (9CI) (CA INDEX NAME)



RN 518058-02-1 HCA
CN 1,7-Heptanediaminium, N,N'-bis[3-(2,5-dioxo-1-pyrrolidinyl)propyl]-N,N,N',N'-tetramethyl- (9CI) (CA INDEX NAME)



RN 518058-06-5 HCA
CN 1,6-Hexanediaminium, N-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-N'-[3-(2,5-dioxo-1-pyrrolidinyl)propyl]-N,N,N',N'-tetramethyl- (9CI) (CA INDEX NAME)



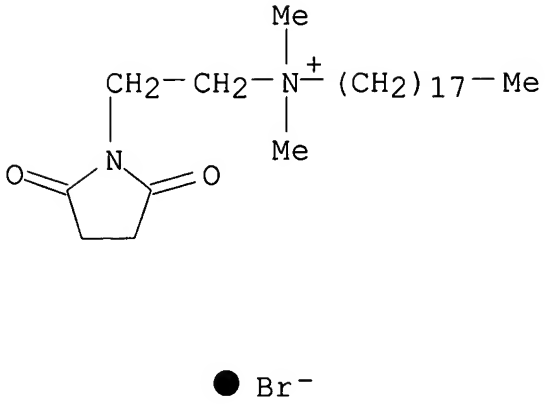
IT **518057-96-0 518057-97-1 518058-02-1**
518058-06-5
(muscarinic M2 receptors modulation by; mapping property distributions of mol. surfaces using algorithm and evaluation of a novel 3D quant. structure-activity relationship technique)

L34 ANSWER 5 OF 30 HCA COPYRIGHT 2006 ACS on STN
133:48261 Synthesis of novel initiators. In situ generation of peroxygenated compounds via the action of sodium percarbonate. Application to the destruction of toxic organophosphorus and sulfur compounds. Lion, Claude; Da Conceicao, Louis; Hedayatullah, Mir (Institut de Topologie et de Dynamique des Systemes de l'Universite Paris 7 Denis Diderot, Associe au CNRS, UPRESA 7086, Paris, 75005, Fr.). Phosphorus, Sulfur and Silicon and the Related Elements, 161, 97-113 (French) 2000. CODEN: PSSLEC. ISSN: 1042-6507. Publisher: Gordon & Breach Science Publishers.

AB New initiators, analogs of tetra-acetylethylenediamine, have been prepd. and their use in the in situ generation of peroxyacids by reaction with sodium peroxycarbonate is described. The kinetics of perhydrolysis of these initiators in aq. soln. under different conditions of temp. and pH, as well as the use of these new "complex peroxygenated systems" in the destruction of organophosphorus and sulfur toxins and pollutants, have been studied.

IT **275824-13-0P**
(synthesis of initiators for in situ generation of peroxygenated compds. via action of sodium percarbonate and their application to destruction of organophosphorus and sulfur compds.)

RN 275824-13-0 HCA
CN 1-Pyrrolidineethanaminium, N,N-dimethyl-N-octadecyl-2,5-dioxo-, bromide (9CI) (CA INDEX NAME)



IT **275824-13-0P**
(synthesis of initiators for in situ generation of peroxygenated compds. via action of sodium percarbonate and their application to destruction of organophosphorus and sulfur compds.)

L34 ANSWER 6 OF 30 HCA COPYRIGHT 2006 ACS on STN
133:12354 Ligands for the common allosteric site of acetylcholine M2-receptors: development and application. Holzgrabe, U.; Bender, W.; Botero Cid, H. M.; Staudt, M.; Pick, R.; Pfletschinger, C.; Balatkova, E.; Trankle, C.; Mohr, K. (Institute of Pharmacy and Food Chemistry, Department of Pharmaceutical Chemistry, University of Wurzburg, Wurzburg, 97074, Germany). Pharmaceutica Acta Helvetiae, 74(2-3), 149-155 (English) 2000. CODEN: PAHEAA. ISSN: 0031-6865. Publisher: Elsevier Science B.V..

AB Ligands for the allosteric site of acetylcholine M2 receptors are able to retard the dissocn. of simultaneously bound ligands for the orthosteric site. This effect promotes receptor occupation by the orthosteric ligand. The allosteric effect opens various therapeutic perspectives, e.g., in organophosphorus poisoning. The aim of our studies was to optimize the affinity of the modulators for the common allosteric binding site of muscarinic M2 receptors, the orthosteric site of which was liganded with the N-methylscolopamine. The phthalimido substituted hexane-bisammonium compd. W84 served as a starting point. Previous mol. modeling studies revealed two pos. charges and two arom. imides in a sandwich-like arrangement to be essential for a high allosteric potency. A three-dimensional quant. structure activity relationship (3D QSAR) anal. predicted compds. with substituents of increasing size on the lateral imide moieties to enhance the affinity for the allosteric binding site. Thus, we synthesized and pharmacol. evaluated compds. bearing "satd." phthalimide moieties as well as phthalimidines with substituents of systematically increasing size in position 3 or on the arom. ring at one or both ends of the mol. Within each series, QSAR could be

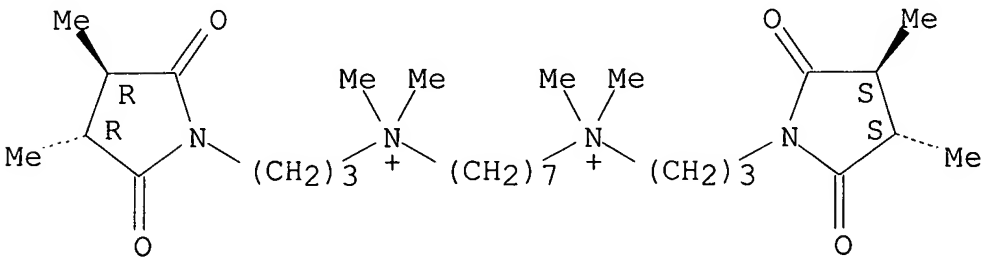
derived. "Satn." of the arom. ring of the phthalimide moiety results in less potent compds. Increasing the size of the substituents in position 3 of the phthalimide enhances the potency. Putting substituents on the arom. part of the phthalimide increases the potency more effectively: the introduction of a Me group in position 5 gave a compd. with a potency in the nanomolar concn. range which was subsequently developed as the first radioligand for the allosteric binding site.

IT **202644-28-8 202644-29-9 202644-30-2 269730-39-4**
(ligands for the common allosteric site of acetylcholine M2-receptors)

RN 202644-28-8 HCA

CN 1,7-Heptanediaminium, N-[3-[(3R,4R)-3,4-dimethyl-2,5-dioxo-1-pyrrolidinyl]propyl]-N'-[3-[(3S,4S)-3,4-dimethyl-2,5-dioxo-1-pyrrolidinyl]propyl]-N,N,N',N'-tetramethyl-, dibromide, rel- (9CI) (CA INDEX NAME)

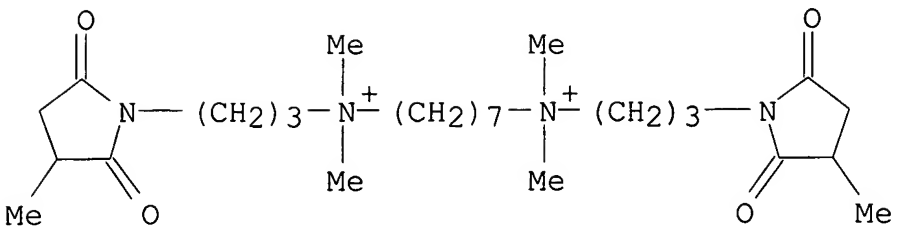
Relative stereochemistry.



●2 Br^-

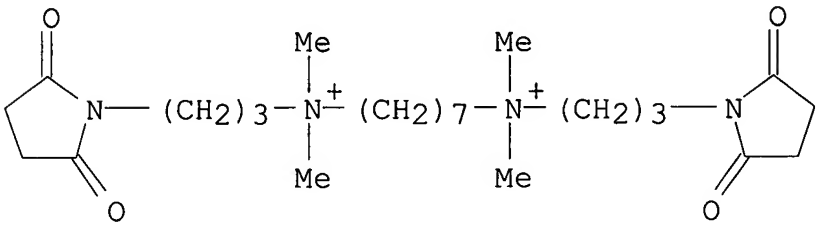
RN 202644-29-9 HCA

CN 1,7-Heptanediaminium, N,N,N',N'-tetramethyl-N,N'-bis[3-(3-methyl-2,5-dioxo-1-pyrrolidinyl)propyl]-, dibromide (9CI) (CA INDEX NAME)



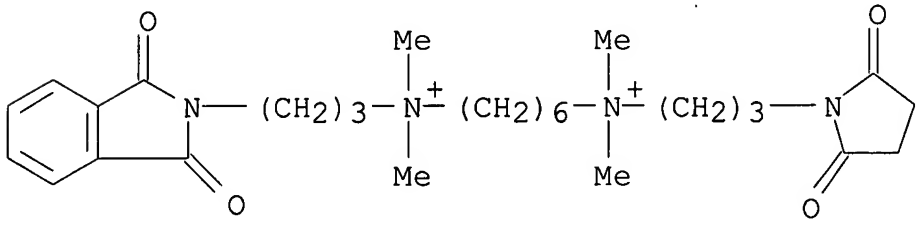
●2 Br^-

RN 202644-30-2 HCA
CN 1,7-Heptanediaminium, N,N'-bis[3-(2,5-dioxo-1-pyrrolidinyl)propyl]-N,N,N',N'-tetramethyl-, dibromide (9CI) (CA INDEX NAME)



●2 Br^-

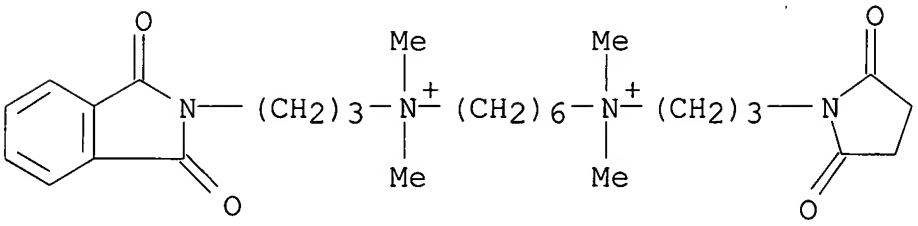
RN 269730-39-4 HCA
CN 1,6-Hexanediaminium, N-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-N'-[3-(2,5-dioxo-1-pyrrolidinyl)propyl]-N,N,N',N'-tetramethyl-, dibromide (9CI) (CA INDEX NAME)



●2 Br^-

IT **202644-28-8 202644-29-9 202644-30-2**
269730-39-4
(ligands for the common allosteric site of acetylcholine M2-receptors)

L34 ANSWER 7 OF 30 HCA COPYRIGHT 2006 ACS on STN
132:342812 Probing the size of a hydrophobic binding pocket within the allosteric site of muscarinic acetylcholine M2-receptors. Bender, Wiebke; Staudt, Markus; Trankle, Christian; Mohr, Klaus; Holzgrabe, Ulrike (Department of Pharmaceutical Chemistry, Institute of Pharmacy, University of Wurzburg, Wurzburg, 97074, Germany). Life Sciences, 66(18), 1675-1682 (English) 2000. CODEN: LIFSAK. ISSN: 0024-3205. Publisher: Elsevier Science Inc..
AB Hexane-bisammonium-type compds. contg. lateral phthalimide moieties are known to have a rather high affinity for the allosteric site of muscarinic M2 receptors. In order to get more insight into the contribution of the lateral substituents for alloster binding affinity, a series of compds. with unilaterally varying imide substituents were synthesized and tested for their ability to retard allosterically the dissocn. of [3H]N-methylscopolamine from the receptor protein (control t1/2 = 2 min; 3 mM MgHCO4, 50 mM Tris, pH 7.3, 37°). Among the test compds., the naphthalimide contg. agent (half max. effect at EC50,diss = 60 nM) revealed the highest potency. Apparently, its affinity for the allosteric site in NMS-occupied receptors is 20fold higher compared with the phthalimide contg. parent compd. W 84. Anal. of quant. structure-activity relationships yielded a parabolic correlation between the vol. of the lateral substituents and the allosteric potency. The maximal vol. was detd. to be approx. 600 Å3 suggesting that the allosteric binding site contains a binding pocket of a defined size for the imide moiety.
IT **269730-39-4P**
(QSAR studies of alkane bisammonium compds. in relation to allosteric binding site on the muscarinic acetylcholine M2-receptors)
RN 269730-39-4 HCA
CN 1,6-Hexanediaminium, N-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-N'-[3-(2,5-dioxo-1-pyrrolidinyl)propyl]-N,N,N',N'-tetramethyl-, dibromide (9CI) (CA INDEX NAME)



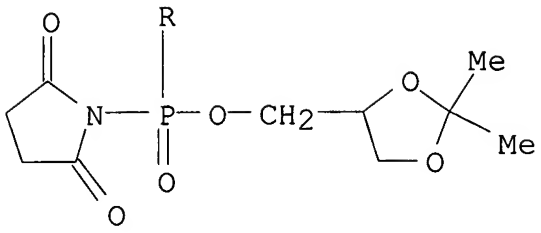
●2 Br^-

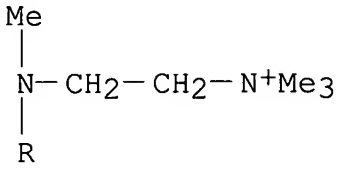
IT **269730-39-4P**
(QSAR studies of alkane bisammonium compds. in relation to allosteric binding site on the muscarinic acetylcholine M2-receptors)

L34 ANSWER 8 OF 30 HCA COPYRIGHT 2006 ACS on STN
131:257634 N-halamides in organophosphorus synthesis. Nifant'ev, E. E.; Predvoditelev, D. A.; Suvorkin, S. V.; Malenkovskaya, M. A.; Bel'skii, V. K. (Moscow State Pedagogical University, Moscow, Russia). Russian Journal of General Chemistry (Translation of Zhurnal Obshchei Khimii), 69(3), 372-377 (English) 1999. CODEN: RJGCEK. ISSN: 1070-3632. Publisher: MAIK Nauka/Interperiodica Publishing.

AB Synthetic potential of reactions of P(III) esters with N-halamides has been evaluated. Exptl. problems in working with the resulting mixed amides have been discussed. Original systems with the nitrogen atom bearing two carbonyl and one phosphoryl substituents have been studied. Phospholipids derived from N-halamides have been synthesized. Thus, reaction of P(OEt)3 with N-bromosuccinimide gave 82% di-Et succinylamidophosphate (1). The crystal structure of succinimide complex of 1 was detd.

IT **245110-63-8P**
(prepn. of)
RN 245110-63-8 HCA
CN Ethanaminium, 2-[[[(2,2-dimethyl-1,3-dioxolan-4-yl)methoxy](2,5-dioxo-1-pyrrolidinyl)phosphinyl]methylamino]-N,N,N-trimethyl-, bromide (9CI) (CA INDEX NAME)





● Br^-

IT **245110-63-8P**
(prepn. of)

L34 ANSWER 9 OF 30 HCA COPYRIGHT 2006 ACS on STN
128:149214 Contribution of lateral substituents in heptane-bisammonium derivatives to the allosteric stabilization of antagonist binding to M2-receptors. Staudt, Markus; Trankle, Christian; Mohr, Klaus; Holzgrabe, Ulrike (Department of Pharmaceutical Chemistry, Institute of Pharmacy, University of Bonn, Bonn, D-53115, Germany). Life Sciences, Volume Date 1998, 62(5), 423-429 (English) 1997. CODEN: LIFSAK. ISSN: 0024-3205. Publisher: Elsevier Science Inc..

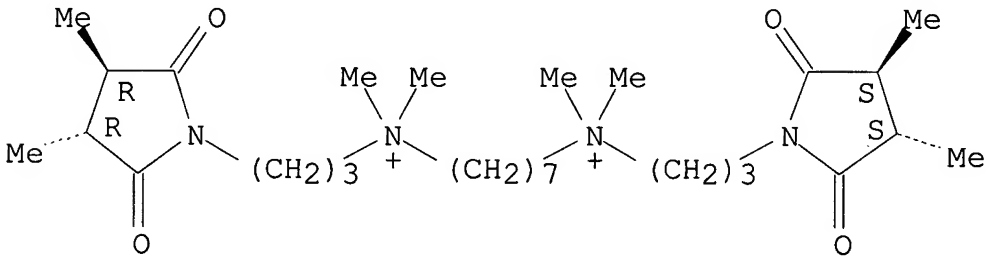
AB Phthalimide-contg. heptane-bisammonium-type compds. retard the dissocn. of the antagonist [3H]-N-methylscopolamine ([3H]NMS) from muscarinic M2-receptor allosterically with high potency. To study the contribution of the lateral substituents to this effect, a series of derivs. was synthesized in which the phthalimide moiety was truncated. The potency of the compds. to delay [3H]NMS dissocn. was measured in porcine heart homogenates (50 mM Tris-HCl, 3 mM MgHPO4, pH 7.3, 37°). Potency declined with diminution of the lateral substituents, e.g. loss of the arom. ring of the phthalimide resulted in a 400 fold redn. in potency. In the hexahydrophthalimide derivs., the cis stereoisomer was about fivefold more potent than the trans-isomer. In conclusion, almost flat hydrophobic lateral moieties appear to be pivotal for high allosteric potency, suggesting a hydrophobic interaction of these parts of the mol. with the [3H]NMS occupied receptor protein.

IT **202644-28-8P 202644-29-9P 202644-30-2P**
(contribution of lateral substituents in heptane-bisammonium derivs. to allosteric stabilization of antagonist binding to M2-muscarinic receptors)

RN 202644-28-8 HCA

CN 1,7-Heptanediaminium, N-[3-[(3R,4R)-3,4-dimethyl-2,5-dioxo-1-pyrrolidinyl]propyl]-N'-[3-[(3S,4S)-3,4-dimethyl-2,5-dioxo-1-pyrrolidinyl]propyl]-N,N,N',N'-tetramethyl-, dibromide, rel- (9CI) (CA INDEX NAME)

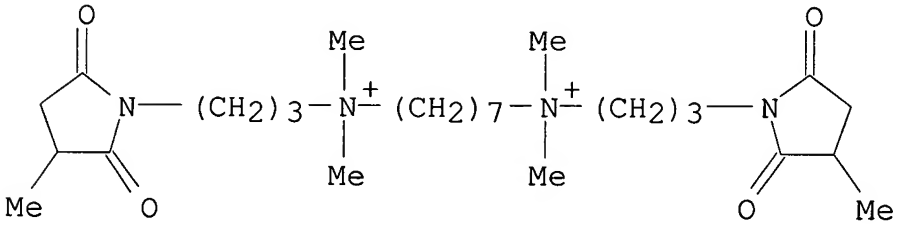
Relative stereochemistry.



● 2 Br^-

RN 202644-29-9 HCA

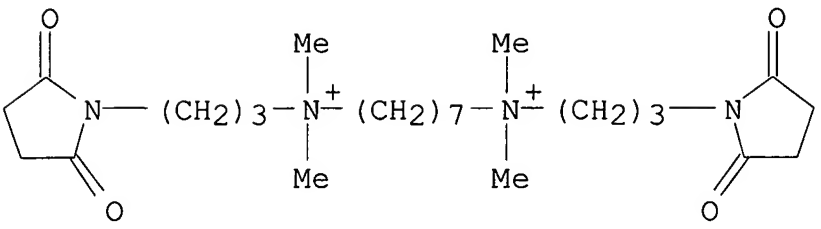
CN 1,7-Heptanediaminium, N,N,N',N'-tetramethyl-N,N'-bis[3-(3-methyl-2,5-dioxo-1-pyrrolidinyl)propyl]-, dibromide (9CI) (CA INDEX NAME)



● 2 Br^-

RN 202644-30-2 HCA

CN 1,7-Heptanediaminium, N,N'-bis[3-(2,5-dioxo-1-pyrrolidinyl)propyl]-N,N,N',N'-tetramethyl-, dibromide (9CI) (CA INDEX NAME)

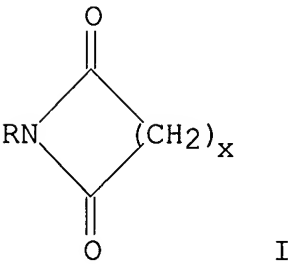


●2 Br^-

IT **202644-28-8P 202644-29-9P 202644-30-2P**
(contribution of lateral substituents in heptane-bisammonium derivs. to allosteric stabilization of antagonist binding to M2-muscarinic receptors)

L34 ANSWER 10 OF 30 HCA COPYRIGHT 2006 ACS on STN
117:10338 Bleaching and detergent compositions containing peroxy acid bleach precursors. Thornthwaite, David William; Oakes, John; Kerr, Colin Watt; Cotter, Byron R. (Unilever N. V., Neth.; Unilever PLC). Eur. Pat. Appl. EP 473229 A1 19920304, 12 pp. DESIGNATED STATES: R: CH, DE, ES, FR, GB, IT, LI, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1991-202144 19910822. PRIORITY: GB 1990-18749 19900828.

GI



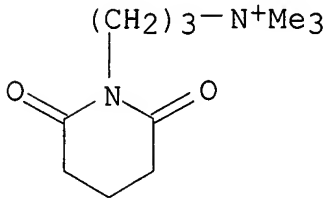
I

AB Cyclic imides I (R = alkyl, quaternary ammonium group-substituted alkyl; x = 2-6) which perhydrolyze to form peroxyacids RNHCO(CH2)xC(O)OOH are useful as bleach activators in laundry detergent compns. contg. peroxygen bleaching agents. A quaternization product of I [R = Me2N(CH2)3; x = 4] and Me2SO4 was used as a bleach activator in the laundry of tea-stained fabrics with a detergent compn. contg. Na perborate monohydrate.

IT **141969-62-2 141969-64-4**
(bleaching activators, for peroxygen compds. in laundering)
RN 141969-62-2 HCA
CN 1-Piperidinepropanaminium, N,N,N-trimethyl-2,6-dioxo-, methyl sulfate (9CI) (CA INDEX NAME)

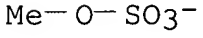
CM 1

CRN 141969-61-1
CMF C11 H21 N2 O2



CM 2

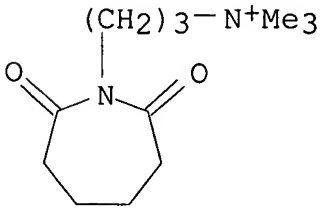
CRN 21228-90-0
CMF C H3 O4 S



RN 141969-64-4 HCA
CN 1H-Azepine-1-propanaminium, hexahydro-N,N,N-trimethyl-2,7-dioxo-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 141969-63-3
CMF C12 H23 N2 O2



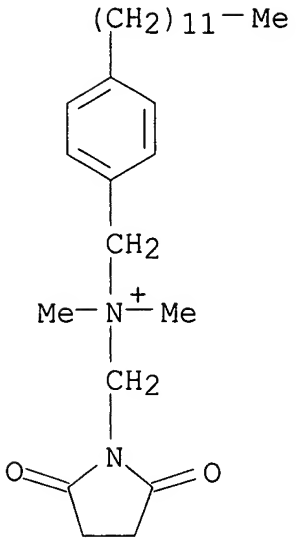
CM 2

CRN 21228-90-0
CMF C H3 O4 S

Me—O—SO_3^-

IT **141969-62-2 141969-64-4**
(bleaching activators, for peroxygen compds. in laundering)

L34 ANSWER 11 OF 30 HCA COPYRIGHT 2006 ACS on STN
115:290877 Potential barriers for electron tunnelling in low-temperature aqueous glasses (comparison of the computer simulation model with experiments). Feret, Blazej; Bartczak, Witold M.; Kroh, Jerzy (Inst. Appl. Radiat. Chem., Tech. Univ., Lodz, Pol.). Radiation Physics and Chemistry, 38(2), 145-8 (English) 1991. CODEN: RPCHDM. ISSN: 0146-5724.
AB The exptl. kinetic data on the trapped electron decay in 6 M NaOH aq. glass doped with electron scavengers were analyzed. The electron decay curves obtained by the computer simulation, assuming simple tunnelling mechanism of the electron transfer, were fitted to the exptl. decays. For a group of scavengers the optimization procedure works well and gives the av. barrier height for electron tunnelling between 1.26 and 1.42 eV. For another group of scavengers, the simple tunnelling mechanism does not provide adequate kinetic model for the trapped electron decay.
IT **1433-24-5**
(electron trapping by, in low temp. aq. glass, computer simulation of kinetics in)
RN 1433-24-5 HCA
CN 1-Pyrrolidinemethanaminium, N-[(4-dodecylphenyl)methyl]-N,N-dimethyl-2,5-dioxo-, chloride (9CI) (CA INDEX NAME)



● Cl^-

IT **1433-24-5**
(electron trapping by, in low temp. aq. glass, computer simulation of kinetics in)

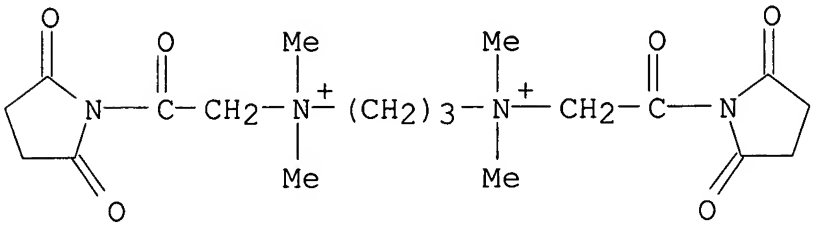
L34 ANSWER 12 OF 30 HCA COPYRIGHT 2006 ACS on STN
115:210692 Novel polycationic compounds as per acid precursors in bleach compositions. Sotoya, Kohshiro; Ogura, Nobuyuki; Imoto, Hiroyuki (Kao Corp., Japan). Eur. Pat. Appl. EP 427224 A1 19910515, 22 pp. DESIGNATED STATES: R: CH, DE, DK, ES, FR, GB, IT, LI, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1990-121290 19901107. PRIORITY: JP 1989-290315 19891108; JP 1990-206396 19900802.

AB ZmX[YX(Zm-1)]nYXZm (n+2)A [X = N+, S+, P+; Y = alkylene, hydroxyalkylene, etc.; Z = YCOB, YO2CB, alkyl, hyroxyalkyl, etc.; ≥1 Z = YCOB or YO2CB; m = 2-3; n = 0-3; A = anionic group; A is absent when X and Z form an inner salt; B = OPh optionally substituted by sulfo, carboxy, OH, etc.), oxime group, imidoxime group, sulfoalkoxy, carboxymethoxy, etc.] are useful as org. per acid precursors in bleach compns. contg. H2O2 or a source or H2O2. A bleaching soln. contg. p-MeOCOC6H4OCO(CH2)3N+(CH2)2N+Me2(CH2)3CO2-p-C6H4CO2Me 2Br- (I) as an activator for Na percarbonate provided better bleaching of tea-stained fabrics than a similar soln. contg. Ac2N(CH2)2NAc2 instead of I.

IT **136861-68-2P**
(prepn. of, for activators for peroxygen bleaching)

RN 136861-68-2 HCA

CN 1,3-Propanediaminium, N,N'-bis[2-(2,5-dioxo-1-pyrrolidinyl)-2-oxoethyl]-N,N,N',N'-tetramethyl-, dichloride (9CI) (CA INDEX NAME)

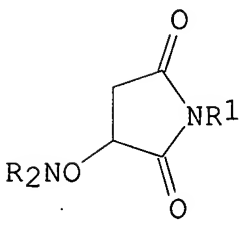


●2 Cl⁻

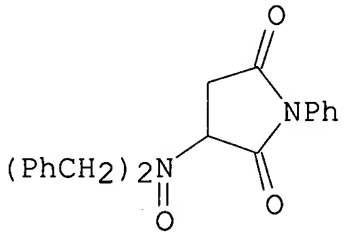
IT **136861-68-2P**
(prepn. of, for activators for peroxygen bleaching)

L34 ANSWER 13 OF 30 HCA COPYRIGHT 2006 ACS on STN
109:230697 Conjugate addition of N,N-dialkylhydroxylamines. Mechanism of O-alkylation by 1H-pyrrole-2,5-diones. Pastor, Stephen D.; Hessell, Edward T. (Addit. Res. Dep., CIBA-GEIGY Corp., Ardsley, NY, 10502, USA). Journal of Organic Chemistry, 53(24), 5776-9 (English) 1988. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 109:230697.

GI



III

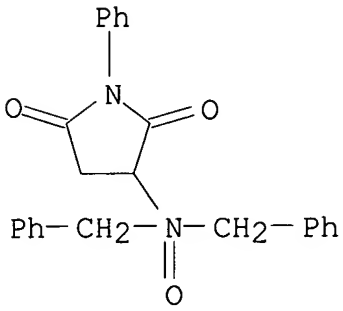


V

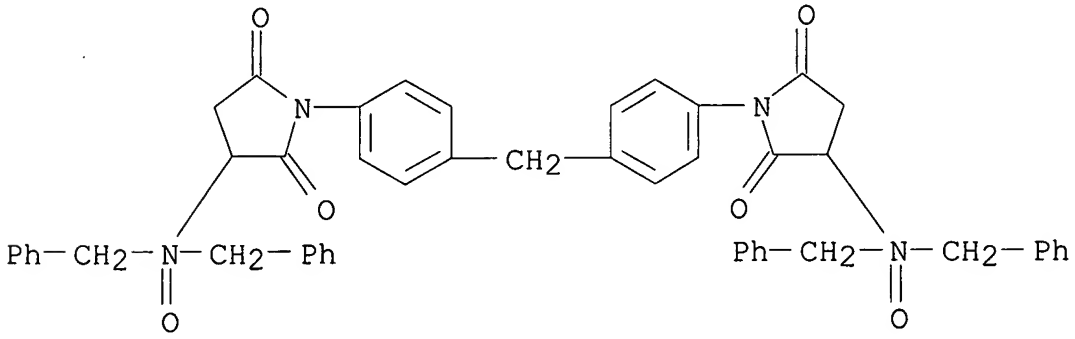
AB Addn. reaction of (PhCH2)2NOH (I) with N-phenylmaleimide (II) in refluxing THF gave O-alkylhydroxylamine III (R = PhCH2, R1 = Ph) (IV) instead of the N-alkyl N-oxide V. Oxidn. of 3-(dibenzylamino)-1-phenyl-2,5-pyrrolidinedione gave Cope elimination products I and II rather than V. This result suggests that IV was formed by direct O-alkylation of I without the intermediacy of V. The reaction of I and II was not inhibited by

the presence of 1.1 equiv m-(O2N)2C6H4; an electron-transfer mechanism is probably not operative. Other III [R = PhCH2, R1 = H, Me, cyclohexyl, (CH2)18H; R = Et, R1 = Ph] were also prepd.

IT **117022-06-7P**
(attempted prepn. of)
RN 117022-06-7 HCA
CN 2,5-Pyrrolidinedione, 3-[oxidobis(phenylmethyl)amino]-1-phenyl- (9CI) (CA INDEX NAME)



IT **117022-09-0P**
(prepn. of)
RN 117022-09-0 HCA
CN 2,5-Pyrrolidinedione, 1,1'-(methylenedi-4,1-phenylene)bis[3-[bis(oxidophenylmethyl)amino]- (9CI) (CA INDEX NAME)



IT **117022-06-7P**
(attempted prepn. of)
IT **117022-09-0P**
(prepn. of)

L34 ANSWER 14 OF 30 HCA COPYRIGHT 2006 ACS on STN
107:190354 Structural requirements for affinity and efficacy of N-(4-amino-2-butynyl)succinimides at muscarinic receptors in the guinea pig ileum and urinary bladder. Ringdahl, Bjorn (Sch. Med., Univ. California, Los Angeles, CA, 90024, USA). European Journal of

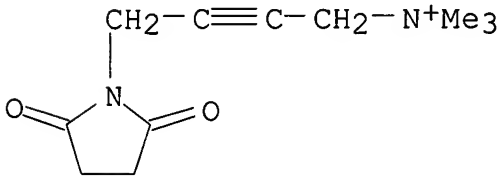
Pharmacology, 140(1), 13-23 (English) 1987. CODEN: EJPHAZ. ISSN: 0014-2999.

AB The muscarinic activities on the isolated guinea pig ileum and urinary bladder of some N-(4-amino-2-butynyl)succinimides, modified only in the amino group, were resolved into receptor affinity and efficacy components. The structural requirements for high affinity and high efficacy were quite different. Cyclic tertiary amino moieties generally favored high affinity, whereas small acyclic amino and ammonium groups favored high efficacy. On the ileum, dissocn. consts. and relative efficacies of the succinimides were highly correlated with those of the identically modified N-(4-amino-2-butynyl)-2-pyrrolidones. This observation suggests that N-(4-manio-2-butynyl)succinimides and 2-pyrrolidones bind to and activate muscarinic receptors in a similar fashion. In spite of their agonist properties on the ileum, the succinimides studied were agonists, partial agonists or competitive antagonists on the urinary bladder. However, dissocn. consts. and relative efficacies of the compds. showed good agreement in the 2 tissues. It therefore appears that muscarinic receptors in the ileum and urinary bladder are pharmacol. similar. The large differences obsd. in agonist potency and relative maximal responses between the 2 tissues were explained by a greater receptor reserve for muscarinic agonists in the ileum than in the bladder.

IT **19433-66-0 110933-11-4 110933-13-6 110933-14-7**
(muscarinic receptor-binding and -agonist activity of, structure in relation to)

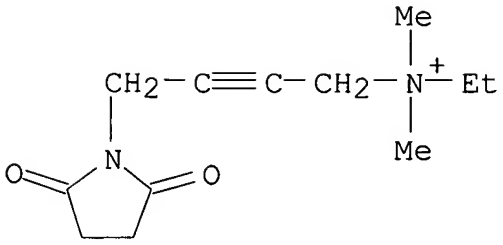
RN 19433-66-0 HCA

CN 2-Butyn-1-aminium, 4-(2,5-dioxo-1-pyrrolidinyl)-N,N,N-trimethyl-, iodide (9CI) (CA INDEX NAME)



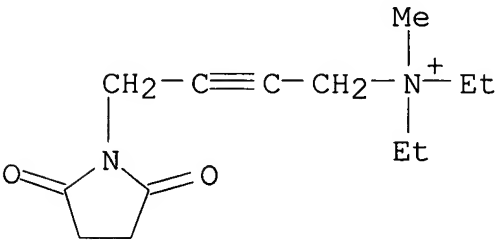
RN 110933-11-4 HCA

CN 2-Butyn-1-aminium, 4-(2,5-dioxo-1-pyrrolidinyl)-N-ethyl-N,N-dimethyl-, iodide (9CI) (CA INDEX NAME)



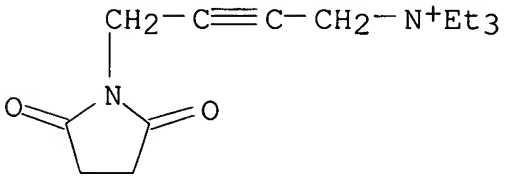
● I^-

RN 110933-13-6 HCA
CN 2-Butyn-1-aminium, 4-(2,5-dioxo-1-pyrrolidinyl)-N,N-diethyl-N-methyl-, iodide (9CI) (CA INDEX NAME)



● I^-

RN 110933-14-7 HCA
CN 2-Butyn-1-aminium, 4-(2,5-dioxo-1-pyrrolidinyl)-N,N,N-triethyl-, iodide (9CI) (CA INDEX NAME)



● I^-

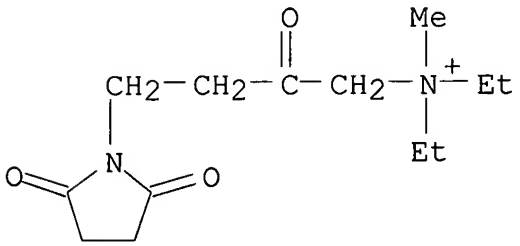
IT **19433-66-0 110933-11-4 110933-13-6**
110933-14-7
(muscarinic receptor-binding and -agonist activity of, structure in relation to)

L34 ANSWER 15 OF 30 HCA COPYRIGHT 2006 ACS on STN
102:24449 Synthesis of some quaternary ammonium alkylating agents and their effects on soman-inhibited acetylcholinesterase. Gray, Allan P.; Platz, Robert D.; Chang, Timothy C. P.; Leverone, Theresa R.; Ferrick, David A.; Kramer, David N. (Dynamac Corp., Rockville, MD, 20852, USA). Journal of Medicinal Chemistry, 28(1), 111-16 (English) 1985. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 102:24449.

AB Eleven quaternary ammonium compds. were prepd. and tested for their ability to realkylate the phosphonate anion of aged, soman-inhibited acetylcholinesterase. None were found able to do so, but [2-(4-pyridyl)ethyl]diethylmethylammonium iodide and its 2-pyridyl isomer slowed the rate of aging significantly.

IT **93185-41-2P**
(prepn. and realkylation by, of phosphonate anion of aged soman-inhibited acetylcholinesterase)

RN 93185-41-2 HCA
CN 1-Pyrrolidinebutanaminium, N,N-diethyl-N-methyl-β,2,5-trioxo-, iodide (9CI) (CA INDEX NAME)



● I^-

IT **93185-41-2P**
(prepn. and realkylation by, of phosphonate anion of aged soman-inhibited acetylcholinesterase)

L34 ANSWER 16 OF 30 HCA COPYRIGHT 2006 ACS on STN
101:225095 Identification of the α subunit half-cystine specifically labeled by an affinity reagent for the acetylcholine receptor binding site. Kao, Peter N.; Dwork, Andrew J.; Kaldany,

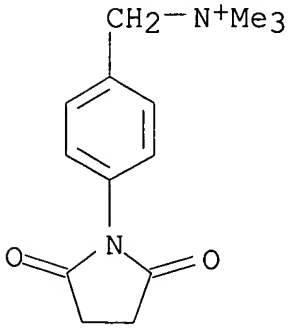
Rashad Rudolf J.; Silver, Michael L.; Wideman, Janusz; Stein, Stanley; Karlin, Arthur (Coll. Physicians Surg., Columbia Univ., New York, NY, 10032, USA). Journal of Biological Chemistry, 259(19), 11662-5 (English) 1984. CODEN: JBCHA3. ISSN: 0021-9258.

AB Nicotinic acetylcholine receptors contain a readily reducible disulfide bond at the periphery of the acetylcholine-binding site. Following redn. of this disulfide, the binding site is susceptible to affinity labeling by electrophilic reagents with quaternary ammonium moieties. Reduced purified receptor from Torpedo californica elec. tissue was affinity alkylated with 4-(N-maleimido)benzyltri[3H]methylammonium iodide. The label was incorporated solely into the α-subunit of the receptor. Isolated, labeled α-subunit was cleaved with CNBr, and the fragments were sepd. by reverse-phase HPLC. A uniquely labeled CNBr fragment was isolated, and its partial sequences was detd. by automated Edman degrdn. This CNBr fragment was cleaved at tryptophan residues, the subfragments were sepd., and the labeled subfragments were partially sequenced. From the protein sequence information, the labeled CNBr fragment was identified as residues 179-207 of the sequence of α predicted from the cDNA sequence. From the cycle of the Edman degrdn. in which radioactive residues were released, it was concluded that cysteine-192 and, possibly in addn., cysteine-193 are the residues specifically labeled by 4-(N-maleimido)benzyltri[3H]methylammonium iodide. They are, therefore, close to the acetylcholine-binding site.

IT **93391-26-5**
(acetylcholine receptor binding site labeling with, site for)

RN 93391-26-5 HCA

CN Benzenemethanaminium, 4-(2,5-dioxo-1-pyrrolidinyl)-N,N,N-trimethyl-, iodide (9CI) (CA INDEX NAME)

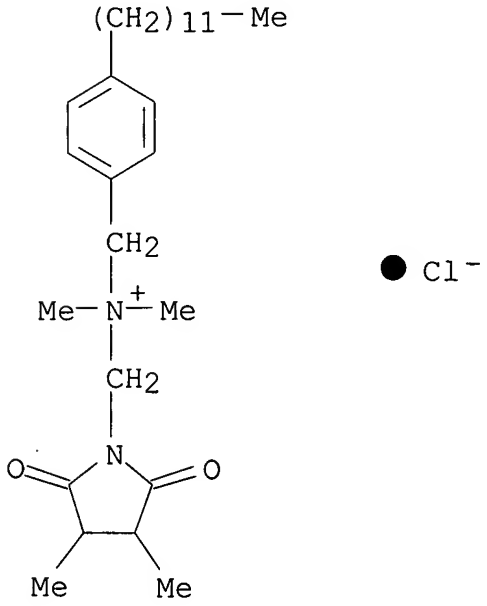


● I^-

IT **93391-26-5**

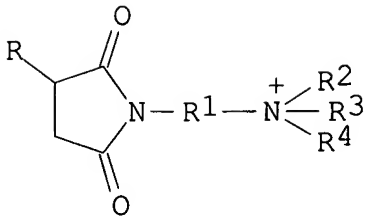
(acetylcholine receptor binding site labeling with, site for)

L34 ANSWER 17 OF 30 HCA COPYRIGHT 2006 ACS on STN
98:82218 The electric dipole moments of OCHF and OCDF. Campbell, E. J.; Read, W. G.; Shea, J. A. (Noyes Chem. Lab., Univ. Illinois, Urbana, IL, 61801, USA). Chemical Physics Letters, 94(1), 69-72 (English) 1983. CODEN: CHPLBC. ISSN: 0009-2614.
AB The elec. dipole moments of the weakly bound complexes CO, HF and CO, DF were measured using pulsed Fourier transform microwave spectroscopy carried in a Fabry-Perot cavity. The results, 2.352(8) D for CO, HF and 2.396(7) D for CO, DF exceed the estd. vector sums of the 2 subunit elec. dipoles by ≈0.55 D in each case.
IT **1433-26-7**
(elec. dipole moment of complex from carbon monoxide and)
RN 1433-26-7 HCA
CN 1-Pyrrolidinemethanaminium, N-[(4-dodecylphenyl)methyl]-N,N,3,4-tetramethyl-2,5-dioxo-, chloride (9CI) (CA INDEX NAME)



IT **1433-26-7**
(elec. dipole moment of complex from carbon monoxide and)

L34 ANSWER 18 OF 30 HCA COPYRIGHT 2006 ACS on STN
92:166259 Fuel composition containing quaternary ammonium salts of succinimides. Vartanian, Paul F. (Texaco Inc., USA). U.S. US 4171959 19791023, 5 pp. (English). CODEN: USXXAM. APPLICATION: US 1977-860545 19771214.
GI



X-

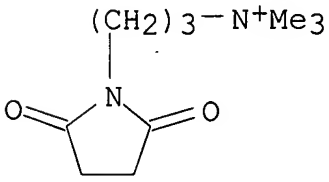
I

AB The cleanliness of carburetors for internal combustion engines is maintained by the use of gasoline contg. 0.005-0.10 wt.% of the quaternary ammonium salt of a succinimide (I; R = hydrocarbyl group of 280-1800 mol. wt.; R1 = C2-10 hydrocarbondiyl; R2, R3 = C1-6 hydrocarbyl or a heterocyclic ring contg. O and (or) N; R4 = C1-6 hydrocarbyl; and X = halide, carboxylate, or sulfonate anion). Thus, a gasoline contg. polyisobutenyl-N-[3-(trimethylammonio)propyl]succinimide iodide (II) [**73343-01-8**] (50 lb additive/1000 bbl fuel) was subjected to the Chevrolet carburetor detergency test in which the ability of the fuel to remove preformed carburetor deposits is measured. The relative effectiveness of the fuel in removing deposits was 70%, whereas the base fuel and the base fuel contg. the succinimide deriv. from which II was derived gave values of -10 and -66%, resp. The performance of the fuel contg. II was comparable to that of premium detergent fuel compns.

IT **73343-01-8 73347-47-4**
(detergent, for gasoline)

RN 73343-01-8 HCA

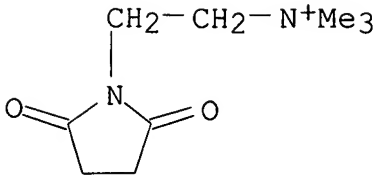
CN 1-Pyrrolidinepropanaminium, N,N,N-trimethyl-2,5-dioxo-, iodide (9CI) (CA INDEX NAME)



● I^-

RN 73347-47-4 HCA

CN 1-Pyrrolidineethanaminium, N,N,N-trimethyl-2,5-dioxo-, iodide (9CI) (CA INDEX NAME)



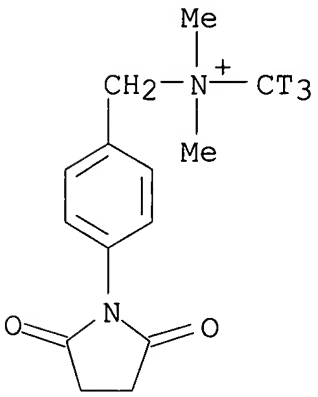
IT **73343-01-8 73347-47-4**
(detergent, for gasoline)

L34 ANSWER 19 OF 30 HCA COPYRIGHT 2006 ACS on STN
89:159078 Characterization of the calcium-binding sites of the purified acetylcholine receptor and identification of the calcium-binding subunit. Ruebsamen, Helga; Eldefrawi, Amira T.; Eldefrawi, Mohyee E.; Hess, George P. (Sect. Biochem., Cornell Univ., Ithaca, NY, USA). Biochemistry, 17(18), 3818-25 (English) 1978. CODEN: BICHAW. ISSN: 0006-2960.

AB The acetylcholine receptor isolated from Torpedo ocellata binds .apprx.8 mol of Tb/mol of α-bungarotoxin-binding sites. This process is accompanied by a fluorescence enhancement of 104 and allows detection of receptor-Tb complexes at μM concns. In the presence of Ca, 2 types of Tb-binding sites are revealed, both with dissocn. consts. (for Tb) in the 18-25 μM range. About 60% of these sites bind Ca with an apparent dissocn. const. of 1 mM. Most of the Tb-binding sites are assocd. with a subunit of the receptor of .apprx.40,000 mol. wt. On the intact mol., the same subunit also reacts with the affinity label p-(N-maleimido)-α-benzyl[trimethyl-3H]ammonium iodide. The Tb-binding sites are preserved when the receptor is degraded by trypsin and chymotrypsin to peptides of mol. wt. ≤8000. These binding sites are, therefore, detd. by structural features of the peptide chain rather than by the 3-dimensional arrangement of the intact receptor. The affinity for Tb in the subunit and the 8000-mol. wt. peptides is the same as in the intact mol. In the subunit and the peptides, all the Tb can be displaced from its binding site by Ca, but the affinity for Ca decreases by a factor of 4 (KCa .apprx.4 mM). Acetylcholine does not interact with the Tb-binding sites in the subunits. In the intact acetylcholine receptor, acetylcholine displaces 3-6 Tb/α-bungarotoxin binding site.

IT **67979-78-6P**
(prepn. of)
RN 67979-78-6 HCA

CN Benzenemethanaminium, 4-(2,5-dioxo-1-pyrrolidinyl)-N,N-dimethyl-N-(methyl-t3)-, iodide (9CI) (CA INDEX NAME)



● I^-

IT **67979-78-6P**
(prepn. of)

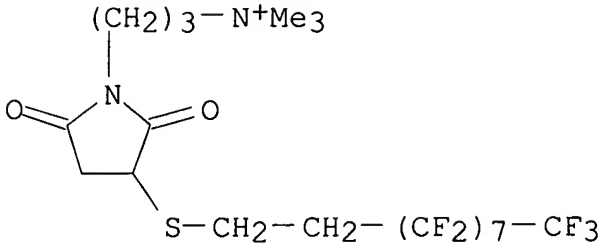
L34 ANSWER 20 OF 30 HCA COPYRIGHT 2006 ACS on STN
85:110392 Perfluoroalkyl group-containing surfactants. Mueller, Karl Friedrich; Falk, Robert A. (Ciba-Geigy A.-G., Switz.). Ger. Offen. DE 2559189 19760708, 139 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1975-2559189 19751230.

AB The surfactants (>20) RCOCHR1CHR1CO2- (I) with R = Me2N+H(CH2)3NH, Me2N+HCH2CH2NMe, Me2N+HCH2CH2O, 2-(quinolium-2-yl)epoxy, or a similar group, 1R1 = C8F17CH2CH2S, C6F13CH2CH2S, or a similar group, and the other R1 = H were pred., as were surface-active succinimides prepd. by ring closure of the I and surface-active quaternary derivs. prepd. from the I and a sultone, alkyl halide, lactone, ect. The surfactants were esp. useful for the prepn. of foams useful for extinguishing burning hydrocarbon liqs. Thus, 10 g maleic anhydride [108-31-6] was treated with Me2N(CH2)3NH2 [109-55-7] and HSCH2CH2C8F17 [34143-74-3] to prep. I (R = Me2N+H(CH2)3NH, 1R1 = C8F17CH2CH2S, and the other R1 = H) [60280-18-4] which gave surface tension 19.8 dynes/cm as a 0.1% aq. soln.

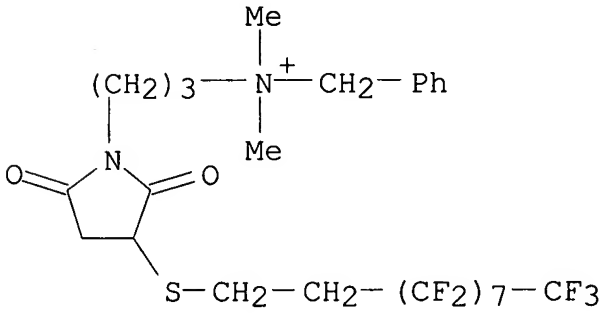
IT **60274-07-9 60274-08-0**
(surfactants, firefighting foams)

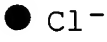
RN 60274-07-9 HCA

CN 1-Pyrrolidinepropanaminium, 3-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)thio]-N,N,N-trimethyl-2,5-dioxo-, iodide (9CI) (CA INDEX NAME)



RN 60274-08-0 HCA
CN 1-Pyrrolidinepropanaminium, 3-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)thio]-N,N-dimethyl-2,5-dioxo-N-(phenylmethyl)-, chloride (9CI) (CA INDEX NAME)





IT **60274-07-9 60274-08-0**
(surfactants, firefighting foams)

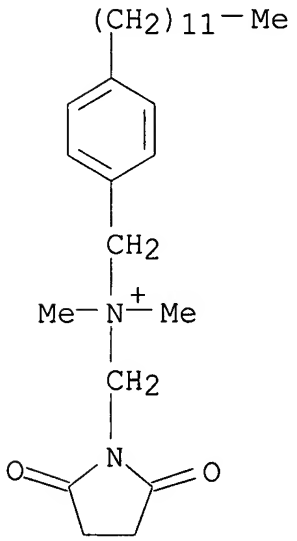
L34 ANSWER 21 OF 30 HCA COPYRIGHT 2006 ACS on STN
83:127870 Anion conductivity of liquid membranes in the presence of valinomycin. Golubev, V. N.; Purins, B. (Inst. Inorg. Chem., Riga, USSR). Biofizika, 20(4), 738-9 (Russian) 1975. CODEN: BIOFAI. ISSN: 0006-3029.
AB Liq. membranes were prepd. by enclosing a layer (.apprx.2 mm thick) of n-heptane contg. 2 + 10-6-2 + 10-3M valinomycin between 2 cellophane membranes, and the permeability of this membrane to ReO4-, MoO42-, and PO4-3 was studied. For ReO4-, the potential difference of the membrane varied linearly with the

logarithm of ReO4- concn. in the concn. range 10-3-10-1M with a slope of 42 mV. Since an ideal membrane has a curve with a slope of 58 mV, the lower value for the liq. membrane indicates the presence of anionic specificity of the membrane. The curves for MoO42- and PO43- had even smaller slopes and the change in the potential difference occurred only for relatively concd. solns. (0.1-2.0M anion). The permeability of the membrane was in the order: ReO4->MoO42->PO43-. In the absence of an applied elec. field, the transport of the anions was very slow and almost nonexistent for MoO42- and PO43-. Application of a field of 450-600 V increased the transport of the anions.

IT **1433-24-5**
(permeation by, of heptane-valinomycin membranes)

RN 1433-24-5 HCA

CN 1-Pyrrolidinemethanaminium, N-[(4-dodecylphenyl)methyl]-N,N-dimethyl-2,5-dioxo-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

IT **1433-24-5**
(permeation by, of heptane-valinomycin membranes)

L34 ANSWER 22 OF 30 HCA COPYRIGHT 2006 ACS on STN

83:61649 Cationic azo dyes from aminohalobenzenesulfonamides. Clark, Gary T. (Eastman Kodak Co.). U.S. US 3836518 19740917, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 1972-233299 19720309.

GI For diagram(s), see printed CA Issue.

AB Cationic azo dyes used for dyeing acrylic fibers fast yellow to

orange shades were prepd. by coupling diazotized 3,4-Cl(H2N)C6H3SO2NHCH2CH2CH2NMe2 (I) [51957-15-4] or 4,3-Cl(H2N)C6H3SO2NHCH2CH2CH2NMe2 (II) [53803-82-0] with N,N-disubstituted aniline derivs., and quaternizing. Thus, 3,4-Cl2C6H3SO2Cl [98-31-7] in Me2CO treated with Me2NCH2CH2CH2NH2 gave 3,4-Cl2C6H3SO2NHCH2CH2CH2NMe2 [53803-83-1], and treatment with NH3 gave I. Diazotization and coupling of II with N-ethyl-N-β-succinimidoethyl-m-toluidine [2498-03-5] gave azo dye intermediate and quaternization with Me2SO4 gave azo dye (III) [**53803-85-3**], orange on acrylic fibers.

IT **53803-85-3P**
(prepn. of)

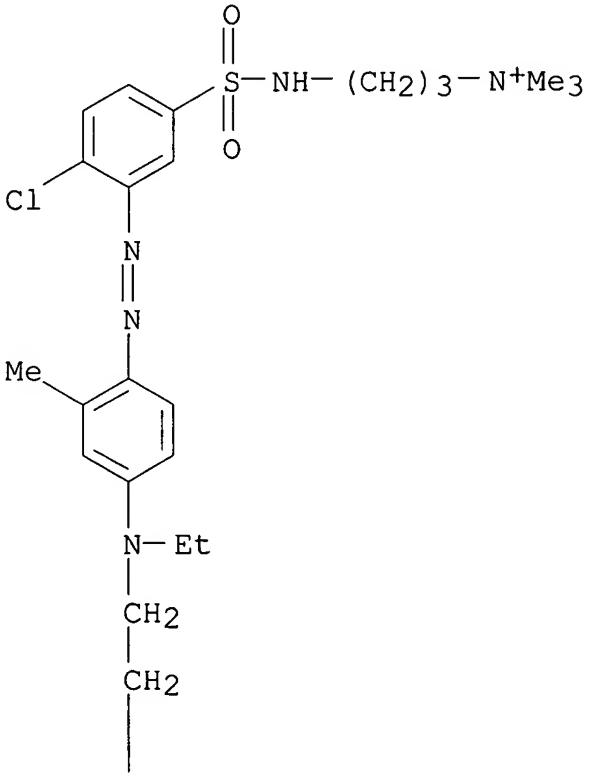
RN 53803-85-3 HCA

CN 1-Propanaminium, 3-[[[4-chloro-3-[[4-[[2-(2,5-dioxo-1-pyrrolidinyl)ethyl]ethylamino]-2-methylphenyl]azo]phenyl]sulfonyl]amino]-N,N,N-trimethyl-, methyl sulfate (9CI) (CA INDEX NAME)

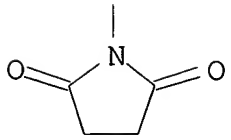
CM 1

CRN 53803-84-2
CMF C27 H38 Cl N6 O4 S

PAGE 1-A



PAGE 2-A



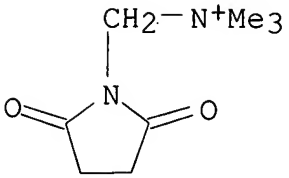
CM 2

CRN 21228-90-0
CMF C H3 O4 S

$Me-O-SO_3^-$

IT **53803-85-3P**
(prepn. of)

L34 ANSWER 23 OF 30 HCA COPYRIGHT 2006 ACS on STN
81:120146 Sulfones as chemical transport forms of germicidal compounds. 5. Synthesis of α-amino and α-amido sulfones.
Messinger, P.; Gompertz, J. (Inst. Pharm. Chem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.). Archiv der Pharmazie (Weinheim, Germany), 307(8), 653-5 (German) 1974. CODEN: ARPMAS. ISSN: 0365-6233.
OTHER SOURCES: CASREACT 81:120146.
AB Reaction of the aminals or amidals RCH(NR1R2)2 (e.g. R = H, Ph, or Me; R1 = H or Me, R2 = Ph, Bz, or Ac or R1R2 = CHPh) with sulfinic acids HSO2C6H4R3-4 (I, R3 = H or Me) gave 40-92% 4-R3C6H4SO2CHRNR1R2. Similarly, reaction of the quaternary compds. RR1NCH2N+-MeR2R4 I- (RR1 = o-COC6H4CO or COCH2CH2CO or R = CHO, R1 = Ph; R2 = R4 = Me or NR2R4 = piperidino) with the Na salts of I gave RR1NCH2SO2C6H4R3-4.
IT **53656-54-5**
(reaction of, with benzenesulfinic acid)
RN 53656-54-5 HCA
CN 1-Pyrrolidinemethanaminium, N,N,N-trimethyl-2,5-dioxo-, iodide (9CI) (CA INDEX NAME)



IT **53656-54-5**
(reaction of, with benzenesulfinic acid)

L34 ANSWER 24 OF 30 HCA COPYRIGHT 2006 ACS on STN
68:103538 Central and peripheral cholinergics and anticholinergics. VII. Structural analogs of oxotremorine, its homologs, and their methiodides. Levy, Jeanne; Michel-Ber, Estera; Fumagalli, Mrs. N.; Gotti, M. B. (Inst. Pharmacol., Paris, Fr.). Therapie, 22(6), 1461-75 (French) 1967. CODEN: THERAP. ISSN: 0040-5957.

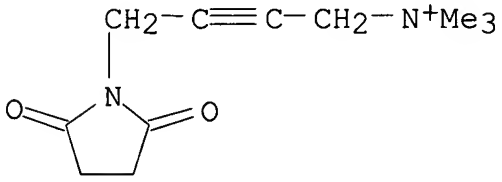
AB Twenty eight amines of general structure XCH2C.tplbond.CCH2Y and 2 methiodides of structure [XCH2C.tplbond.CCH2NMe3]+I- were examd. for peripheral and central nervous system activity in mice. Of 21 compds. with X = 2,5-dioxopyrrolidin-1-yl, 2,6-dioxopiperidino, or benzo[c]2,5-dioxopyrrolidin-1-yl (1,3-dioxoisoindolin-1-yl) groups examd. on rat duodenum, the compd. with X = 2,5-dioxopyrrolidin-1-yl and Y = pyrrolidin-1-yl (I) had spasmogenic cholinergic activity, while 8 compds., including those with X = 2,5-dioxopyrrolidin-1-yl, Y = piperidino (II) and X = 2,5-dioxopyrrolidin-1-yl, Y = hexahydroazepino (III), were weakly anticholinergic. The two methiodides, with X = 2,5-dioxopyrrolidin-1-yl or X = 2,6-dioxopiperidino, had peripheral cholinergic activity. Of 7 other amines tested, X = 3-methyl-5-ethyl-5-phenyl-2,4,6-trioxohexahydropyrimidin-1-yl, Y = piperidino; X = 3,5-dimethyl-5-(1-cyclohexene-1-yl)-2,4,6-trioxohexahydropyrimidin-1-yl, Y = pyrrolidin-1-yl; and X = N-acetyl-N-methylamino, Y = piperidino (IV) had weak peripheral anticholinergic activity. II, III, IV, and the compd. with X = 2,6-dioxopiperidino, Y = hexahydroazepino were the most active central anticholinergics in mice, while I and the compd. X = 2,5-dioxopyrrolidin-1-yl, Y = NMe2 had central cholinergic activity. Of the 28 amines, the central cholinergic and anticholinergic activity of those with X = 2,5-dioxopyrrolidin-1-yl and Y = pyrrolidin-1-yl, piperidino, hexahydroazepino, or octahydroazocino showed the greatest pharmacol. similarity to oxotremorine or oxotremorine homologs.

IT **19433-66-0 19433-67-1**

(nervous system response to)

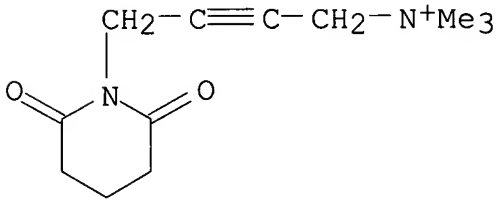
RN 19433-66-0 HCA

CN 2-Butyn-1-aminium, 4-(2,5-dioxo-1-pyrrolidinyl)-N,N,N-trimethyl-, iodide (9CI) (CA INDEX NAME)



RN 19433-67-1 HCA

CN Ammonium, (4-glutarimido-2-butynyl)trimethyl-, iodide (8CI) (CA INDEX NAME)



IT **19433-66-0 19433-67-1**

(nervous system response to)

L34 ANSWER 25 OF 30 HCA COPYRIGHT 2006 ACS on STN

68:94574 Effect of muscarinic agents on the thermoregulatory centers in the rat. Kirkpatrick, W. E.; Lomax, Peter; Jenden, Donald J. (Sch. of Med., Univ. of California, Los Angeles, CA, USA). Proceedings of the Western Pharmacology Society, 10, 51-5 (English) 1967. CODEN: PWPSA8. ISSN: 0083-8969.

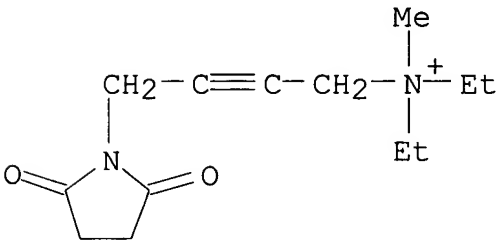
AB Intracerebral injection of carbachol into rats produced a hypothermic response. Both systemic administration as well as injection into the thermoregulatory centers of oxotremorine induced a hypothermic response. N-[4-(Diethylamino)-2-butynyl]succinimide-HCl (DKJ 21), an analog of oxotremorine with anticholinergic

properties, prevented the hypothermic effect of oxotremorine. DKJ itself increased core temp. Systemic N-[4-(diethylamino)-2-butynyl]succinimide methobromide (KS 18) could not block the hypothermic response of oxotremorine, while central administration did block the response. This was because of its failure to cross the blood-brain barrier. Both systemic administration of atropine as well as injection into the thermoregulatory centers abolished the hypothermic response of oxotremorine. Intracerebral administration of atropine increased core temp. Thermoregulatory centers contain muscarinic receptors.

IT **19487-81-1**
(inhibition of hypothermia from oxotremorine by)

RN 19487-81-1 HCA

CN 2-Butyn-1-aminium, 4-(2,5-dioxo-1-pyrrolidinyl)-N,N-diethyl-N-methyl-, bromide (9CI) (CA INDEX NAME)



● Br

IT **19487-81-1**
(inhibition of hypothermia from oxotremorine by)

L34 ANSWER 26 OF 30 HCA COPYRIGHT 2006 ACS on STN

62:8966 Original Reference No. 62:1604a-c Pesticides. Lo, Chien-Pen; Orsage, Richard L. (Rohm & Haas Co.). DE 1141130 19621213, 5 pp. (Unavailable). PRIORITY: US 19590828.

GI For diagram(s), see printed CA Issue.

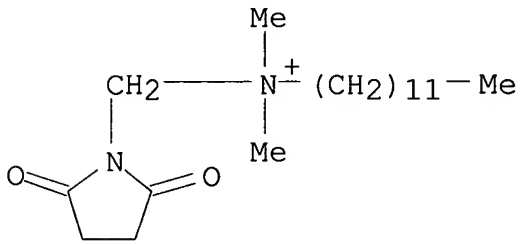
AB Antiseptic-fungicidal agents (I), safe for tender plants and effective for sterilizing equipment used in their culture are prepd. by adding a tertiary amine to N-chloromethylsuccinimide. A soln. of dodecenylsuccinimide 105 and 37% CH2O 36 in dioxane 200 parts was boiled 3 hrs., evapd. at reduced pressure, then dried by azeotropic distn. with benzene to yield 108 crude hydroxymethylimide. Chlorination with SOCl2 gave an oil, b0.2 151-73°. n25D 1.4962. A mixt. of N-chloromethylsuccinimide 12, dodecyldimethylamine 17.3, and acetone 80 parts was boiled 2.5 hrs. to give II, m. 171-3% 23 parts. Similarly prepd. compds. (R1, R2

both Me, R = H), R3 and m.p. given, were: CH2CH:CHCH2CMe2CH2CMe3. 188-90°; CH2-C6H4C12H25, 193-4°; CH2CH2OCH2CH2OC6H4CH2CMe2CH2C-Me3, 154-7°; CH2C6H4C12H25, R = C12H23, oil; CH2Ph, R = C12H23, 161-3°; CH2C6H4C12H25, from sym-dimethylsuccinic acid, oil.

IT **1433-22-3**, Ammonium, dodecyldimethyl(succinimidomethyl), chloride **1433-24-5**, Ammonium, (p-dodecylbenzyl)dimethyl(succinimidomethyl), chloride **1433-25-6**, Ammonium, dimethyl(succinimidomethyl)[2-[2-[p-(1,1,3,3-tetramethylbutyl)phenoxy]etboxy]ethyl], chloride **1433-26-7**, Ammonium, [(2,3-dimethylsuccinimido)methyl](p-dodecylbenzyl)dimethyl, chloride **1447-51-4**, Ammonium, dodecyldimethyl(succinimidomethyl), bromide **31426-56-9**, 1-Pyrrolidinemethanaminium, 3-(dodecenyl)-N-[(4-dodecylphenyl)methyl]-N,N-dimethyl-2,5-dioxo-, chloride **31605-71-7**, Ammonium, benzyl[[2-(dodecenyl)succinimido]methyl]dimethyl-, chloride
(prepn. of)

RN 1433-22-3 HCA

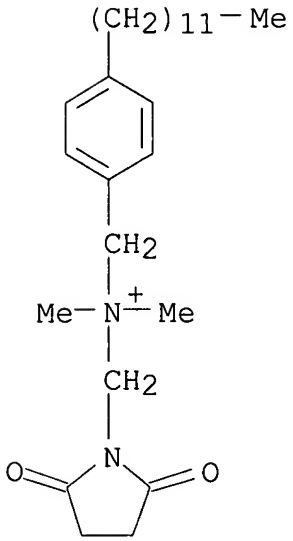
CN Ammonium, dodecyldimethyl(succinimidomethyl)-, chloride (8CI) (CA INDEX NAME)



● Cl^-

RN 1433-24-5 HCA

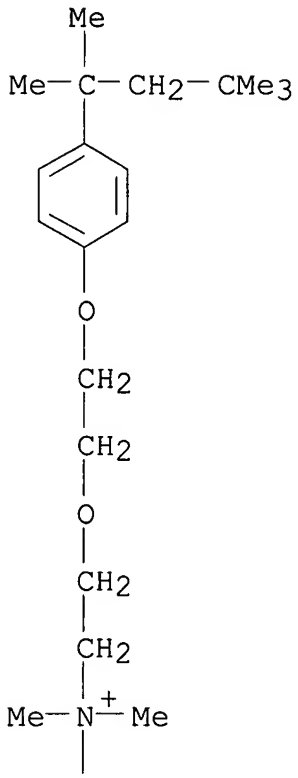
CN 1-Pyrrolidinemethanaminium, N-[(4-dodecylphenyl)methyl]-N,N-dimethyl-2,5-dioxo-, chloride (9CI) (CA INDEX NAME)



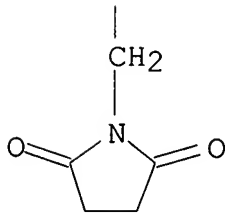
● Cl^-

RN 1433-25-6 HCA
CN Ammonium, dimethyl(succinimidomethyl)[2-[2-[p-(1,1,3,3-tetramethylbutyl)phenoxy]ethoxy]ethyl]-, chloride (8CI) (CA INDEX NAME)

PAGE 1-A

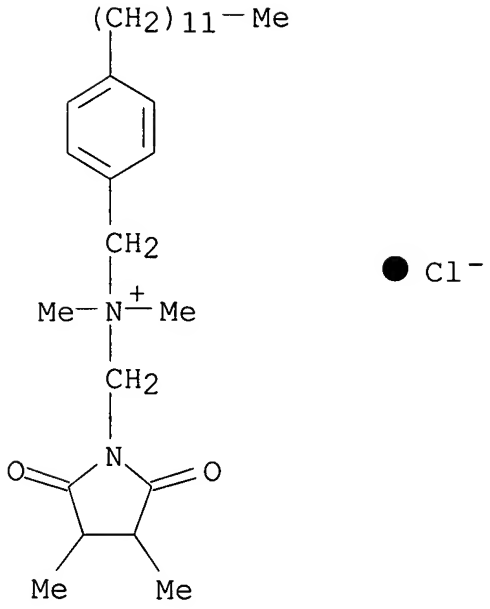


PAGE 2-A

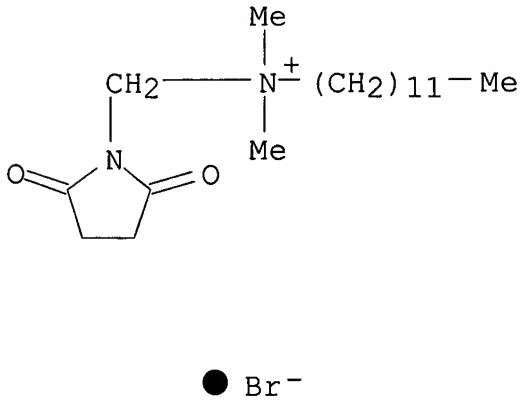


● Cl^-

RN 1433-26-7 HCA
CN 1-Pyrrolidinemethanaminium, N-[(4-dodecylphenyl)methyl]-N,N,3,4-tetramethyl-2,5-dioxo-, chloride (9CI) (CA INDEX NAME)



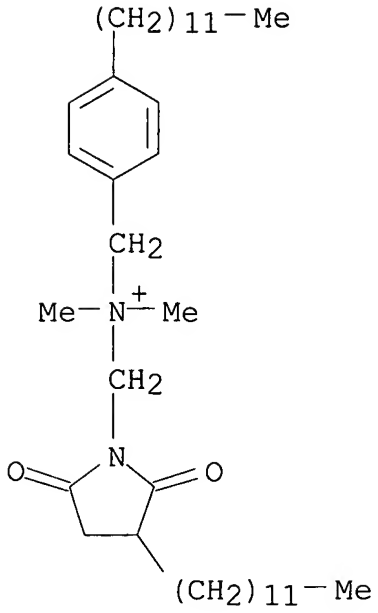
RN 1447-51-4 HCA
CN Ammonium, dodecyldimethyl(succinimidomethyl)-, bromide (8CI) (CA INDEX NAME)



RN 31426-56-9 HCA
CN 1-Pyrrolidinemethanaminium, 3-(dodecenyl)-N-[(4-dodecylphenyl)methyl]-N,N-dimethyl-2,5-dioxo-, chloride (9CI) (CA INDEX NAME)

CM 1

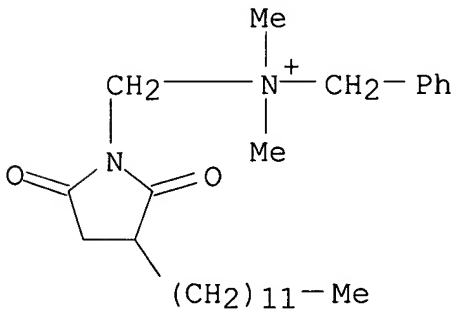
CRN 54514-84-0
CMF C38 H67 N2 O2



RN 31605-71-7 HCA
CN Ammonium, benzyl[[2-(dodecenyl)succinimido]methyl]dimethyl-, chloride (8CI) (CA INDEX NAME)

CM 1

CRN 47656-76-8
CMF C26 H43 N2 O2



IT **1433-22-3**, Ammonium, dodecyldimethyl(succinimidomethyl), chloride **1433-24-5**, Ammonium, (p-dodecylbenzyl)dimethyl(succinimidomethyl), chloride **1433-25-6**, Ammonium, dimethyl(succinimidomethyl)[2-[2-[p-(1,1,3,3-tetramethylbutyl)phenoxy]etboxy]ethyl], chloride **1433-26-7**, Ammonium, [(2,3-dimethylsuccinimido)methyl](p-dodecylbenzyl)dimethyl, chloride **1447-51-4**, Ammonium, dodecyldimethyl(succinimidomethyl), bromide **31426-56-9**,

1-Pyrrolidinemethanaminium, 3-(dodecenyl)-N-[(4-dodecylphenyl)methyl]-N,N-dimethyl-2,5-dioxo-, chloride **31605-71-7**, Ammonium, benzyl[[2-(dodecenyl)succinimido]methyl]dimethyl-, chloride
(prepn. of)

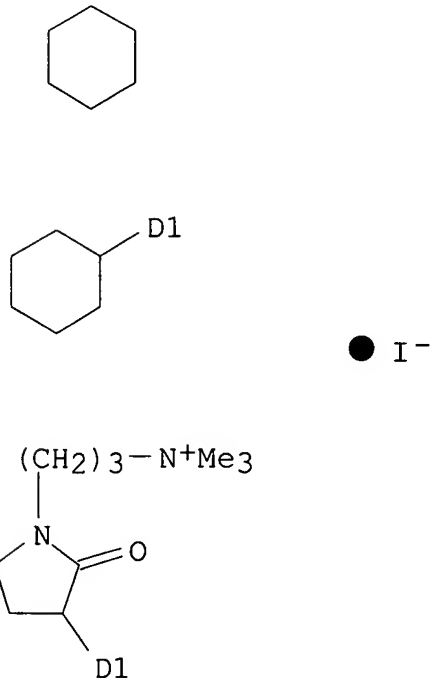
L34 ANSWER 27 OF 30 HCA COPYRIGHT 2006 ACS on STN
60:30809 Original Reference No. 60:5450a-b N-Alkylation of 2- and 4-carbamoylpyridine. Hjedo, Hans (Roy. Danish School Pharm., Copenhagen). Acta Chemica Scandinavica, 17(8), 2351 (English) 1963. CODEN: ACHSE7. ISSN: 0904-213X.

AB 1,1'-Trimethylenebis(4-carbamoylpyridinium bromide)-2H2O, m. 256-7°, was prepd. by heating iso-nicotinamide and 1,3-dibromopropane in EtOH 1 hr. at 120° in an autoclave. The corresponding chloride, m. 263-4°, was prepd. from the bromide and freshly pptd. AgCl. 2-Carbamoyl-1-methylpyridinium iodide, m. 171-2°, was prepd. with α-picolinamide and MeI. The corresponding chloride, m. 223-4°, was prepd. from the iodide in H2O with freshly pptd. AgCl.

IT **101123-40-4**, [3-([Bicyclohexyl]-4,4-diacetimido)propyl]trimethylammonium iodide
(prepn. of)

RN 101123-40-4 HCA

CN [3-([Bicyclohexyl]-4,4-diacetimido)propyl]trimethylammonium iodide (7CI) (CA INDEX NAME)



IT **101123-40-4**, [3-([Bicyclohexyl]-4,4-diacetimido)propyl]trimethylammonium iodide
(prepn. of)

L34 ANSWER 28 OF 30 HCA COPYRIGHT 2006 ACS on STN
58:66529 Original Reference No. 58:11375b-h,11376a-h,11377a-h,11378a-e
Photographic light-sensitive silver halide-polyvinyl alcohol emulsions. Sprung, Joseph A. (General Aniline & Film Corp.). DE 1139738 19621115, 44 pp. (Unavailable). PRIORITY: US 19590119.

AB Photographic poly(vinyl alc.)-Ag halide emulsions with predetd. and predictable properties can be prepd. by regulating the elec. charge on the surface of the Ag halide grains. This distribution and regulation of the charges can be achieved by enveloping the light-sensitive grains with certain surface-active agents or activating agents which will be adsorbed by the surface of the Ag halide crystals. The desired distribution of the elec. charges can be achieved by producing the photographic poly(vinyl alc.) emulsions in the presence of various ampholytic surface-active agents or mixts. of ampholytic and cationic surface-active agents. The cationic surface-active substances useful in this invention contain at least 8 C atoms in an aliphatic chain which is substituted by groups as primary, secondary, and tertiary amino, quaternary ammonium, NHNH2, azonium, guanyl, guanido, biguanido, amine oxide, ternary sulfonium, or quaternary phosphonium. The surface-active ampholytic substances of this invention are obtained by the introduction of CO2H, SO3H, SO2H, OSO3H, PO3H2, PO2H2, OPO3H2, O2PO2H, SH, or OH groups into the cationic agents. Since the photographic activity of the light-sensitive grains is closely related to the type of pos. charge, a series of Ag halide emulsions with various photographic properties can be obtained by a change of structure of the cationic agent. However, Ag halide emulsions sensitized with cationic surface-active agents exhibit a tendency towards fogging, requiring thus a relatively large amt. of added stabilizer or the addnl. use of surface-active ampholytic agents. A series of cationic, surface-active agents was prepd. Paraformaldehyde (66 g.) in 170.5 g. hot 90% HCO2H treated with stirring with 213 g. C14H29NH2 in 500 cc. C6H6, stirred 0.5 hr., heated to boiling, cooled, treated with stirring with 187 g. 85% KOH in 325 cc. MeOH, and stirred (0.5 hr., and the C6H6 layer kept overnight over NaOH pellets and distd. yielded 184.7 g. C14H29NMe2, b0.06-0.07 115-25°. Br(CH2)10Br (I) with 2 mole equivs. (CH2NH2)2 yielded H2N(CH2)14NH2. I (0.1 mole) treated with 0.2 mole morpholine in EtOH, filtered, and distd. gave 1,10-dimorpholinodecane. Bu2NH and I gave similarly [Bu2N(CH2)5]2, b15, 109-15°. Et2NH (1.2 mole) and 0.2 mole I in C6H6 refluxed, filtered, and distd. gave [Et2N(CH2)5]2, b1 142-5°. C10H21CH(NH2)CO2H (II) heated with EtOH satd. with dry HCl yielded C10H21CH(NH2)CO2Et.HCl, m. 67° (EtOH-petr. ether). Me ester

of II in MeOH satd. with NH3, kept 5 days, and evapd. yielded C10H21CH(NH2)CONH2.HCl, m. 90-1° (aq. MeOH). Me2NCH2CO2Me (0.342 mole), 1.0 g. Na2CO3, and 0.31 g. C16H33NH2 (III) heated several hrs. at 220°, cooled, and poured into H2O, and the org. layer distd. yielded C16H33NHCOCH2NMe2, m. 48-9°, b0.05-0.09 165-80°. ClCH2CO2Na (0.5 mole) and 2.4 moles Et2NH refluxed several hrs. and evapd., the residue treated with 0.5 mole III in 230 cc. MeOH, the EtOH distd., and the residue heated 3 hrs. at 240° and distd. yielded C16H33NHCOCH2NEt2, b0.05 172-5°. C7H17CO2H (0.3 mole) and 0.33 mole Me2N(CH2)3NH2 (IV) heated 0.5 hr. at 200-30° and distd. gave C7H15CONH(CH2)3NMe2, b0.6 155-6°. In the same manner were prepd. the following RCONH(CH2)3NMe2 (R and b.p./mm. given): C9H19 175-8°/2, C11H23 195-204°/1, C13H27 173-8°/0.09, C15H31, 194-7°/0.08 (m. 57-8°), C17H35 (V) [m. 62-4° (Me2CO)]. C14H29Br with 2 mole equivs. PhCH2NH2 gave C14H20NHCH2Ph. [HO2C(CH2)4]2 (0.2 mole) and 0.4 mole IV refluxed 2 hrs. in 100 cc. dry C6H6 and filtered yielded [(CH2)4CONH(CH2)3NMe2]2, m. 100-2° (C6H6). C17H35COCl and Et2NCH2CH2NH2 heated 0.5 hr. at 200-30° gave C17H35CONH(CH2)2NEt2, m. 61-2°. 6-Aminoquinoline (0.05 mole) and 0.05 mole myristoyl halide in 25 cc. C5H5N heated 2 hrs. on the steam bath and poured into H2O yielded N-(6-quinolyl)myristamide, m. 90-1° (EtOH-petr. ether). 2-Aminopyridine gave similarly N-(2-pyridyl)myristamide. C8H17NH2 (0.1 mole) and 0.1 mole S-methylisothiouronium p-toluenesulfonate in 25 cc. EtOH refluxed 6 hrs. gave [C8H17NHC(:NH)NH3][p-MeC6H4SO3], m. 82-3° (Me2CO). In the same manner were prepd. the following compds. [RNHC(:NH)NHO3][p-MeC6H4SO3] (R and m.p. given): C10H21, 94-5°; C12H25, 103°; C14H29, 76-80°; C16H33, 79-85°; C18H37, 87-91°; p-C14H29OC6H4, 88-9°. [C12H25NH3[p-MeC6H4SO3](0.67 mole) and 0.66 mole dicyandiamide (VI) in 50 cc. HCONMe2 refluxed 3.5 hrs., treated with 12.5 g. CuSO4.5H2O in 50 cc. HCONMe2, and filtered, and the residue heated with AcOH yielded [C12H25NH[C(:NH)NH]2H][p-MeC6H4SO3], m. 217-18° (MeOH). III gave similarly C16H33NH[C(:NH)NH]2H [p-MeC6H4SO3], m. 208-10°. Polyoxymethylene (15 g.) and 0.5 mole PhNH2 in 300 cc. 95% EtOH, the resulting solid, m. 137-8°, probably the polymeric anil, treated with 0.2 mole VI in 100 cc. H2O and 16.4 cc. concd. HCl, refluxed 0.5 hr., and treated with aq. alkali, and the ppt. repptd. from AcOH with Me2CO gave [H2N[C(:NH)NH]2C6H4CH2]n. p-MeC6H4SO3Me (VII) (0.033 mole) and 0.03 mole C16H33NMe2 (VIII) in 100 cc. Me2CO refluxed 2 hrs., cooled, dild. with Et2O, and filtered gave [C16H33NMe3][p-MeC6H4SO3], m. 223-9° (decompn.). C18H37NBu2 with VII gave [C18H37NBu2Me][p-MeC6H4SO3], m. 69-70°. VIII with BrCH2CO2Et yielded [C16H33NMe2CH2CO2Et]Br, m. 54-6°. By quaternization with VII were prepd. in the usual manner the following compds. [RCONH(CH2)3NMe3] [p-MeC6H4SO3H]

(R and m.p. given): C7H15, 132-4°; C9H19, 89-91°; C11H23, 86°; C15H31, 110-11°; C17H35, 111-12°. C15H31CONH(CH2)3NMe2 with ClCH2CONH2 gave [C15H31CONH(CH2)3NMe2CH2CONH2]Cl, m. 89-90°. C15H31CONH(CH2)3NMe2 (IX) with BrCH2CO2Et yielded [C15H31CONH(CH2)3NMe2CH2CO2Et]Br, m. 62-4°. IX with Br(CH2)3CO2Et gave [C15H31CONH(CH2)3NMe2(CH2)3CO2Br]Br, m. 62-5°. C17H35CONHCH2CO2H, m. 120-2°, from C17H35COCl with H2NCH2CO2H heated with HCl-MeOH, and the resulting Me ester, m. 78°, treated with IV yielded C17H35CONHCH2CONH(CH2)3NMe2 (X), m. 97-9°. N-(3-Dimethylaminopropyl)-α-decenyl succinimide (XI) with EtBr gave XI.EtBr, m. 170-2°. N-(3-Dimethylaminopropyl)-succinimide (XII) and C18H37NHOCCH2Br gave the quaternary salt, m. 187-8°. XII with C16H33Br yields XII.C16H33Br, m. 160-2°. AcNH(CH2)3NMe2 with p-MeC6H4SO3C16H33 gave [AcNH(CH2)3NMe2C16H33][p-MeC6H4SO3], m. 134-5°. N-(3-Dimethylaminopropyl)-α-octadodecenylsuccinimide (XIII) with PhCOCH2Br gave the quaternary salt. C16H33NHCOCH2NMe2 (XIV) with VII yielded [C16H33NHCOCH2NMe3][p-MeC6H4SO3], m. 112-13°. C16H33NHCOCH2NEt2 (XV) with PhCH2Br gave [C16H33NHCOCH2NEt2CH2Ph]Br, m. 140-1°. XIV with BzCH2Br yielded [C16H33NHCOCH2NMe2CH2Bz]Br, m. 142-4°. XV with BrCH2CO2Et gave [C16H33NHCOCH2NEt2CH2CO2Et]Br, m. 71-3°. XV with Br(CH2)3CO2Et yielded [C16H33NHCOCH2NEt2(CH2)3CO2Et]Br, m. 37-8°. p-C16H33OC6H4CONH(CH2)3NMe2 with VII gave [p-C16H33COC6H4CONH(CH2)3NMe3][p-MeC6H4SO3], m. 126-7°. p-C15H31CONHC6H4CONH(CH2)3NMe3 (XVI) with VII yielded [p-C15H31CONHC6H4CONH(CH2)3NMe3][p-MeC6H4SO3] (XVII), m. 150°. The m-isomer of XVI gave similarly the m-isomer of XVII, m. 155°. C16H33Br with C5H5N gave [C5H5NC16H33]Br, m. 58-9°. C5H5N and p-MeC6H4SO3C18H37 yielded [C5H5NC18H37][p-MeC6H4SO3], m. 129-30°. C10H21CHBrCONH2 and C5H5N gave [C5H5NCH(CONH2)C10H21]Br, m. 147-8°. N-Octylnicotamide and VII yielded [3-C8H17NHCOC5H4NMe][p-MeC6H4SO3], m. 104°. N-Decylnicotamide and VII gave [3-C10H21NHCOC5H4NMe] [p-MeC6H4SO3H], m. 112-13°. In the same manner were prepd. the following compds. (m.p. given): [3-C12H25NHCOC5H4NMe] [p-MeC6H4SO3], 116°, [3-C16H33NHCOC5H4NMe][p-MeC6H4SO3], 110-11°, [3-C16H33NHCOC5H4NCH2Ph]Br, 95-7°, [3-C16H33NHCOC5H4NCH2CO2Et]Br, 106-7°, [3-EtO2CC5H4NC16H33]Br, m. 101-2°. 2-Methylbenzothiazole with p-MeC6H4SO3C18H37, gave the quaternary salt, m. 137-8°. Me2NNH2 (XVIII) (1 mole) and 0.5 mole (C12H25Br heated in EtOH yielded [C12H25NMe2NH2]Br, m. 156-61°. XVIII with p-MeC6H4SO3C16H33 yielded [C16H33NMe2NH2][p-MeC6H4SO3] (XIX), m. 178-80°. XVII and p-MeC6H4SO3C18H37 gave [C18H37NMe2NH2]-[p-MeC6H4SO3], m. 177-9°. XIX heated 15 hrs. on the steam bath with Ac2O gave

the N-Ac deriv. of XIX, m. 75-6°. C15H33CONHNMe2 (XX) (0.05 mole) and 0.1 mole VII heated 5 hrs. on the steam bath, and the product repptd. from Me2CO with dry Et2O yielded [C15H13CONHNMe3] [p-MeC6H4SO3], m. 100-2°. C17H33CONHNMe2 gave similarly [C17H35CONHMe3] [p-MeC6H4SO3], m. 113-14°. XX and BrCH2CO2Et gave [C15H33CONHNMe2CH2CO2Et]Br, m. 129-30°. VIII (0.01 mole) and 0.01 mole 2-chlorobenzothiazole (XXI) heated 7 hrs. on the steam bath, the mixt. ground with Et2O, cooled, and filtered, and the residue repptd. from hot Me2CO with Et2O gave dimethylhexadecyl(2-benzothiazolyl)ammonium chloride, m. 225-6°. C17H35CONH(CH2)3NMe2 (0.01 mole) and 0.02 mole XXI heated 12 hrs. on the steam bath yielded 2-benzothiazolyldimethyl(3-stearoylaminopropyl)ammonium chloride. 2-Chloroquinoline (0.02 mole) with 0.01 mole VIII yielded 2-quinolyldimethylhexadecylammoniu m chloride, m. 228-30°. C16H33SO2Cl (XXII) (0.02 mole) and 0.033 mole XVIII yielded C16H33SO2NHNMe2 (XXIII), m. 66-7°. XXIII (0.005 mole) and 0.01 mole VIII heated 1 hr. on the steam bath, the crude mixt. ground with Et2O and filtered, and the residue repptd. from hot Me2CO with Et2O yielded [C16H33SO2NHNMe3][p-MeC6H4SO3], m. 105-6°. C14H29SEt (0.04 mole) and 0.04 mole MeI heated 6 hrs. on the steam bath gave [C14H29SEtMe]I, m. 70-1° (95% EtOH-Et2O). XXII, m. 49-50°, and IV in refluxing C6H6 yielded C16H33SO2NH(CH2)3NMe2 (XXIV), m. 68-9° (petr. ether). XXIV with VII yielded [C16H33SO2NH(CH2)3NMe3][p-MeC6H4SO3], m. 125°. p-C11H23CONHC6H4SO2NH(CH2)3NMe2, m. 77-8°, from p-C11H23CONHC6H4SO3Cl and IV treated with VII gave [p-C11H23CONHC6H4SO2NH(CH2)3NMe3] [p-MeC6H4SO3], m. 77-8°. A series of ampholytic, surface-active substances was prepd. C12H25NH2 (0.1 mole) and 0.1 mole BrCH2CO2Na in 20 cc. 50% EtOH refluxed 8 hrs. and evapd., and the residue recrystd. from MeOH-Me2CO gave C15H25NHCH2CO2H. Similarly were prepd. C16H33NHCH2CO2H and C18H37NHCH2CO2H. C16H33NH2 with BrCH2CH2CO2Na yielded C16H33NHCH2CH2CO2H. N-Hexadecyl-2-pyrrolidone (0.038 mole) and 20 cc. concd. HBr in 50 cc. H2O refluxed 26 hrs., cooled, and filtered gave C16H33NH(CH2)3CO2H. H2N(CH2)5CO2H.HBr (0.03 mole), 0.03 mole C14H29Br, and 0.06 mole NaOH in 5 cc. H2O and 25 cc. EtOH refluxed 4 hrs. gave C14H29NH(CH2)5CO2H. Equimolar amts. ClCH2CO2Na and C18H37NHMe in MePh heated 11 hrs. on the steam bath yielded Me(C18H37)NCH2CO2H. C10H21CHBrCO2H (XXV) heated 3 hrs. at 58° with concd. NH4OH contg. traces of (NH4)2CO3 yielded C10H21CH(NH2)CO2H (XXVI), m. 263° (AcOH). Poly-(1-vinyl-2-pyrrolidone) (0.1 mole), 90 cc. 40% HBr, and 120 cc. H2O refluxed 20 hrs. and evapd. in vacuo, and the residue repptd. from EtOH with Me2CO yielded (CH2CH)nNH(CH2)3CO2H. BrCH2CO2Na (0.2 mole) and 0.1 mole C16H33NH2 in EtOH refluxed yielded C16H33N(CH2CO2H)2, decomp. 160° (aq. EtOH and Me2CO). BrCH2CO2Na and XXVI (0.02 mole each) in aq. MeOH refluxed and evapd. gave C10H21CH(CO2H)NHCH2CO2H. BrCH2CO2Na (0.3 mole) and 0.1 mole

H2NCH2CH2NHC12H23 in aq. MeOH refluxed yielded C10H21N(CH2CO2H)CH2CH2N(CH2CO2H)2. XXV (0.1 mole) and 0.3 mole H2NCH2CH2OH in aq. MeOH refluxed 5 hrs. gave C10H21CH(CO2H)NHCH2CH2OH. C10H21CH(NH2)CONHCH2CO2H, m. 174-5% was prepd. by the method of Hopewood and Waizman, (CA 5, 2853). BzNH(CH2)4CHBrCO2H condensed with C16H33NH2, and the product hydrolyzed with 40% HBr yielded H2N (CH2)4CH(CO2H)NHC16H33. C10H21CH(NH2)CONHCH(CO2H)CH2CO2H, m. 108° was prepd. by the method of (CA JCS 99, 1584(1911)). XIII hydrolyzed with NaOH in MeOH gave C18H35CH(CO2H)CH2CONH(CH2)3NMe2. BrCH2CO2H (30.6 g.) in 200.0 cc. MeOH, 59.5 g. C18H37NMe2 in MeOH, and 9.1 g. NaOH in 200.0 cc. MeOH refluxed 2 hrs. and evapd., the residue triturated with boiling Me2CO and filtered, and the crude product dissolved in 175.0 cc. hot iso-PrOH, filtered, cooled, and dild. with a little Me2CO gave 69.0 g. C16H33Me2N+CH2CO2-. BrCH2CO2H (30.6 g.) in 200.0 cc. MeOH, 73.8 g. V in MeOH, and 9.1 g. NaOH in 200.0 cc. MeOH yielded similarly 75.0 g. C17H35CONH(CH2)3N+Me2CH2CO2-. BrCH2CO2H (2.3 g.), 6.38 g. X, and 0.68 g. NaOH in MeOH gave C17H35CONHCH2CONH(CH2)3N+Me2CMe2CO2-. BrCH2CONHCH2CO2H (XXVII) (8.63 g.), 11.9 g. C18H37NMe2, and 1.82 g. NaOH in MeOH yielded. C16H33N+Me2CH2CONHCH2CO2-. XXVII (43.1 g.), 73.6 g. V, and 9.1 g. NaOH in 500.0 cc. MeOH gave 103.0 g. C15H31CONH(CH2)3N+Me2CH2COCH2CH 2CO2-. Succinic anhydride (50.0 g.) and 56.0 g. IV heated at 200-20° yielded XII, b0.07, 108-10°. XII (7.35 g.), 12.2 g. C16H33Br, and 100.0 cc. Me2CO refluxed 15 hrs., cooled, and filtered yielded dimethylhexadecyl(3-succinimidopropyl)ammonium bromide (XXVIII), m. 160-2° (Me2CO). XXVIII (9.78 g.) and 0.83 g. NaOH in 25.0 cc. MeOH refluxed 8 hrs. and evapd., the residue triturated with boiling iso-PrOH and filtered, and the filtrate evapd. gave 8.8 g. C16H33N+Me2(CH2)3NHCOCH2CH2CO2-. Octadecenylsuccinic anhydride with EtBr gave similarly EtMe2N+(CH2)3NHCOCH2CH(C18H35)CO2-. C16H33SO3Na (64.0 g.), 40.5 g. PCl5, and 100.0 cc. POCl3 refluxed 3 hrs. gave 18.0 g. XXII, m. 49-50°. XXII (24.5 g.) and 30.9 g. IV in 400.0 cc. dry C6Ht? heated 2 hrs. on the steam bath, cooled, and shaken with aq. NaHCO3, and the org. phase worked up yielded 18.0 g. C16H33CONH(CH2)3NMe3 (XXIX), m. 68-9°. XXIX condensed with BrCH2CO2H yielded C16H33SO2NH(CH2)3N+Me2CH2CO2-, m. 113-14°. C14SEt with ClCH2CO2H yielded C14EtS+CH2CO2-. Arginine-HCl and C11H23COCl (XXX) (1 equiv. each) heated with 2 equivs. NaOH yielded H2N(HN:)CNH(CH2)3CH(CO2H)NHCOC11H23, m. 200-5°. [C16H33Me2NCH2CH2Br]Br (XXXI) heated with excess aq. Na2SO3 yielded C16H33N+Me2CH2CH2SO3- XXXI with Na2S2O3 in EtOH gave similarly C16H33Me2N+CH2CH2S2O3- . p-C11H23CONHC6H4SO2NH(CH2)3NMe2 with BrCH2CO2H yielded p-C11H23CONHC6H4SO2NH(CH2)3N+Me2CH2CO2-, m. 210-12°. A series of substances useful as antifogging agents and stabilizers in this invention was prepd. o-C6H4(NH2)2 and C11H23CO2H heated at 150-200° gave 2-undecylbenzimidazole, m.

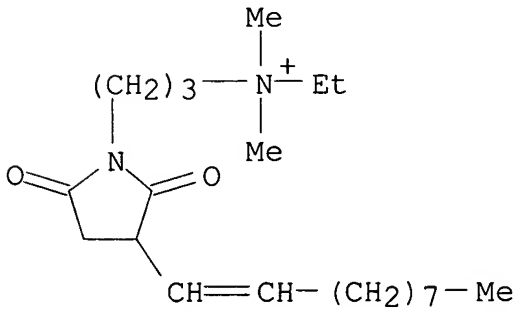
107°. 2-Aminobenzimidazole and C13H27COCl (XXXII) in Me2CO treated with excess Et3N gave 2-lauroylaminobenzimidazole. Histidine-HCl and XXXII in Et2O with Et3N gave the α-tetradecanoylamino analog, m. 112° (aq. MeOH). Histidine Me ester-HCl and XXXII (equimolar amts.) in CHCl3 heated with Et3N gave the α-tetradecanoyl analog, m. 118-19°. 5-Aminotetrazole (XXXIII) treated with excess C9H19COCl (XXXIV) in dry C5H5N-CHCl3 yielded 5-C9H19CONH analog of XXXIII, m. 224-5° (95% EtOH). XXXIII with a slight excess XXXII gave similarly the 5-C13H27CONH analog of XXXIII, m. 220° (abs. EtOH). Na2S2O3 and BrCH2CONHC18H37 (equimolar amts.) yielded C8H37NHCOCH2S2O3Na, m. 175-80° (decompn.) (abs. EtOH). 6-Amino-2-mercaptobenzothiazole (XXXV) in aq. NaOH treated with a slight excess of XXXIV yielded the 6-C9H19CONH analog of XXXV, m. 165-6° (PHCl). XXXV with XXX gave the 6-C11H23CONH analog of XXXV, m. 171-2° (PHCl). 5-Amino-2-mercaptobenzimidazole with XXXIV yielded similarly the 5-C9H19CONH analog, m. 257-61° (MeOH), and with XXX the 5-C11H23CONH analog, m. 266-7°. 2-Chloro-5-lauroylaminoquinoline (XXXVI) and CS(NH2)2 in abs. EtOH refluxed gave the yellow cryst. 5-lauroylamino-2-mercaptoquinoline (XXXVII), m. 225-7°. Similarly was prepd. the 8-C11H23CONH isomer of XXXVII, m. 141-3°. 1-Chloro-5-lauroylaminoisoquinoline with CS(NH2)2 refluxed in abs. EtOH and then treated with alkali gave the 1-SH analog, m. 218-19° (decompn.). C13H27CO2Et and excess CS(NH2)2 refluxed in abs. EtOH with excess NaOEt yielded 4-tridecyl-5-hydroxy-2-mercaptopyrimidine, m. 145° (C6H6). L-Cystine in aq. NaOH treated with excess C7H15CO2H yielded [SCH2CH(CO2H)NHCOC7H15]2, m. 99-100° (petr. ether-EtOAc). L-Cysteine with XXX gave similarly [SCH2CH(CO2Et)NHCOC11H23]2 (XXXVIII), m. 112-13° (EtOH-Et2O-petr. ether). Di-Et cystinate in dry C6H6 with 2 mole equivs. XXX in the presence of C5H5N yielded [SCH2CH(CO2Et)2NHCOC11H23]2, m. 97-8° (abs. EtOH). 2-Chloromethyl-5-nitrobenzimidazole and VIII in abs. EtOH refluxed gave the quaternary salt, m. 196-7° (abs. EtOH). 3-Bromoacetamido-1,2,4-triazole and VIII heated in Me2CO gave the quaternary salt, m. 165° (Me2CO). 4(5)-(Chloromethyl)-imidazole-HCl and 2 mole equivs. VIII refluxed in abs. EtOH gave the quaternary salt, m. 195° (abs. EtOH). C12H25CHBrCO2H with 3 equivs. aq. KOH refluxed gave C12H25CH(OH)CO2H, m. 79-80° (CHCl3-petr. ether), m. 79-80°. 4,2-H2N(HO)C6H3CO2H and a slight excess of XXXII in dry C6H6 yielded 4,2-C13H27CONH(HO)C6H3CO2H, m. 138° (95% EtOH). AgNO3 (10.0 g.) in 70.0 cc. H2O added at 50° during 1-30 min. to 150.0 g. 12.0% aq. Gelvatol 2/75, 40.0 cc. 10% aq. NaCl, 10.0 cc. 0.01M ampholyte soln., and 8.0 cc. 0.01 M aq. soln. of a cationic compd., the mixt. digested 0.5 hr. at 50°, a 100.0-g. portion treated with 1.0-10.0 cc. 0.05% optically sensitizing dye soln., 0.6-1.2 cc.

0.5%-0.1% aq. stabilizer, 1.6 cc. 8.0% aq. saponin, and H2O, and the mixt. coated on paper gave a photographic contact paper comparable to com. gelatin emulsion contact papers. AgNO3 (10.0 g.) in 50.0 cc. H2O added during 1-30 min. at 50° to 150.0 g. 12.0% Gelvatol 2/75, 13.0 cc. 50.0% aq. KBr, 4.5 cc. 10.0% aq. NaCl, 0.0-0.5 cc. 10.0% aq. KI, 5.0-10.0 cc. 0.01M ampholyte soln., and 2.0 cc. 0.01M cationic agent soln., digested 0.5 hr. at 50°, a 100.0-g. portion treated with 1.0-5.0 cc. 0.001M aq. Na2S2O3, 2.0-5.0 cc. 0.01M aq. [SCH2CH(CO2H)NHCOC11H23]2, or another stabilizer, 1.6 cc. 8.0% aq. saponin, and H2O, and coated on paper gave a photographic paper for projection copies. Similar examples for the production of washed emulsions of the ammonia-type, and of highly sensitive neg. emulsions of the boiled type by means of poly(vinyl alc.) are given.

IT **856317-98-1**, Ammonium, [3-(decenylsuccinimido)propyl]ethyldimethyl, bromide **856586-89-5**, Ammonium, dimethyl[3-(octadecenylsuccinimido)propyl]phenacyl, bromide
(prepn. of)

RN 856317-98-1 HCA

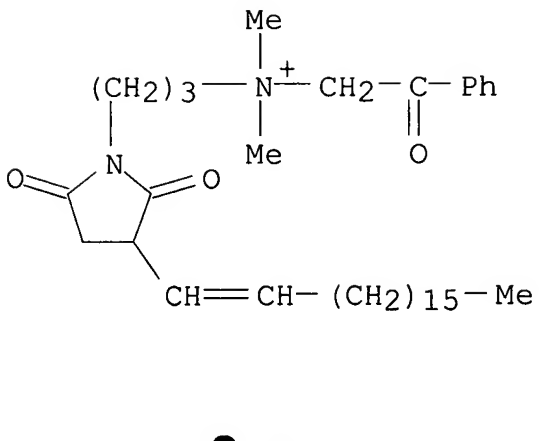
CN Ammonium, [3-(decenylsuccinimido)propyl]ethyldimethyl, bromide (7CI) (CA INDEX NAME)



● Br^-

RN 856586-89-5 HCA

CN Ammonium, dimethyl[3-(octadecenylsuccinimido)propyl]phenacyl, bromide (7CI) (CA INDEX NAME)



IT **856317-98-1**, Ammonium, [3-(decenylsuccinimido)propyl]ethyldi methyl, bromide **856586-89-5**, Ammonium, dimethyl[3-(octadecenylsuccinimido)propyl]phenacyl, bromide (prepn. of)

L34 ANSWER 29 OF 30 HCA COPYRIGHT 2006 ACS on STN

56:52996 Original Reference No. 56:9979d-e,9980a-e N-Succinimidomethyl-substituted quaternary ammonium compounds. Lo, Chien-Pen; Orsage, Richard L. (Rohm & Haas Co.). US 3017416 19620116 (Unavailable). APPLICATION: US 19590828. PRIORITY: US 19590828.

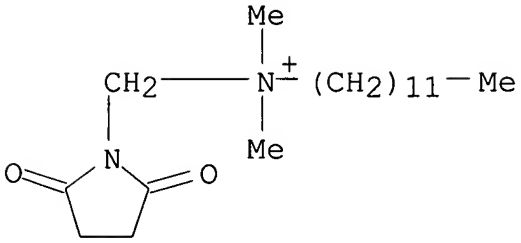
AB Quaternary ammonium compds. contg. the N-succinimidomethyl group, in which the succinimide ring may be alkyl- or alkenyl-substituted and one of the remaining groups on the quaternary N atom is a lipophilic group of 10-25 C atoms, were prepd. by the reaction of a N-halomethylsuccinimide with the appropriate tertiary amine at 25-150°, with or without solvent. Thus, N-chloromethylsuccinimide (I) 12, dodecyldimethylamine 17.3, and acetone 80 parts were refluxed 2.5 hrs. The solid product was washed with addnl. acetone and air-dried to give dodecyldimethyl(succinimidomethyl)ammonium chloride 23 parts, m. 171-3° (decompn.). Similarly, I and N-octadecylmorpholine gave octadecyl(succinimidomethyl)morpholinium chloride; I 12 and dimethyl(5,5,7,7-tetramethyl-2-octenyl)amine 17.2 gave dimethyl(succinimidomethyl)-5,5,7,7-tetramethyl-2-octenylammonium chloride 24, m. 188-90° (decompn.); I 14.8 and (p-dodecylbenzyl)dimethylamine (II) 30.3 gave (p-dodecylbenzyl)dimethyl(succinimidomethyl)ammonium chloride 35.2, m. 193-4° (decompn.); I and N-dodecylbenzylpyrrolidine gave dodecylbenzyl(succinimidomethyl)pyrrolidinium chloride; I and N-dodecylpiperidine gave dodecylbenzyl(succinimidomethyl)piperidiniu m chloride; I 14.8 and p-tert-octylphenoxyethoxyethyldimethylamine

32.2 gave dimethyl(p-tert-octylphenoxyethoxyethyl)succinimidomethyla mmonium chloride 38.1 parts, m. 154-7° (decompn.). In other examples, (N-chloromethyl)-α-dodecenylsuccinimide (III) 13.5 and II 5.8 gave benzyl(α-dodecenylsuccinimidomethyl)dimethylam monium chloride 5.3, m. 161-3°; III 15 and (p-dodecylbenzyl)dimethylamine 14.5 gave oily (α-dodecenylsuccinimidomethyl) (p-dodecylbenzyl)dimethylammonium chloride 25; III 31.4 and N-methylmorpholine (IV) 10.1 gave oily (α-dodecenylsuccinimidomethyl)methylmorpholinium chloride 40; N-chloromethyl-α-dodecylsuccinimide (V) and II gave (α-dodecylsuccinimidomethyl)(p-dodecylbenzyl)dimethylammonium chloride; V and IV gave oily (α-dodecylsuccinimidomethyl)methy lmorpholinium chloride; and N-chloromethyl-α,α'-dimethylsuccinimide (VI) 8 and II 14.4 gave oily (p-dodecylbenzyl)dimethyl(α,α'-dimethylsuccinimidomethyl)ammonium chloride 15.5 parts. III, b0.2 151-73°, n25D 1.4962, and VI (oil) were prepd. by the treatment of α-dodecenylsuccinimide and α,α'-dimethylsuccinimide, resp., with HCHO to give the N-hydroxymethyl derivs. which were treated, resp., with SOCl2 to give the N-chloromethyl compds. Dodecylbenzyldimethyl(α-methylsuccinimidomethyl)ammonium chloride was also claimed. The (succinimidomethyl)ammonium compds. of the invention were found to have fungicidal activity with low phytotoxicity toward growing plants.

IT **1433-22-3**, Ammonium, dodecyldimethyl(succinimidomethyl), chloride **1433-24-5**, Ammonium, (p-dodecylbenzyl)dimethyl(succinimidomethyl), chloride **1433-26-7**, Ammonium, [(2,3-dimethylsuccinimido)methyl](p-dodecylbenzyl)dimethyl, chloride **31426-56-9**, 1-Pyrrolidinemethanaminium, 3-(dodecenyl)-N-[(4-dodecylphenyl)methyl]-N,N-dimethyl-2,5-dioxo-, chloride **31605-71-7**, Ammonium, benzyl[[2-(dodecenyl)succinimido]methyl]dimethyl-, chloride **106336-73-6**, Ammonium, dimethyl(succinimidomethyl)[2-[2-[p-(2,2,4,4-tetramethylpentyl)phenoxy]ethoxy]ethyl], chloride
(prepn. of)

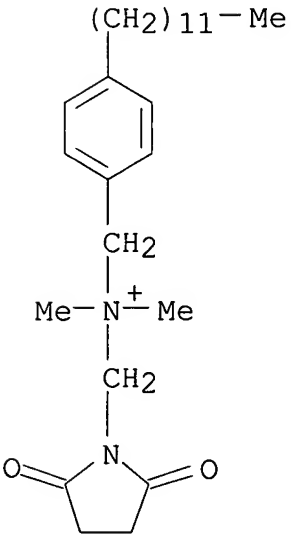
RN 1433-22-3 HCA

CN Ammonium, dodecyldimethyl(succinimidomethyl)-, chloride (8CI) (CA INDEX NAME)



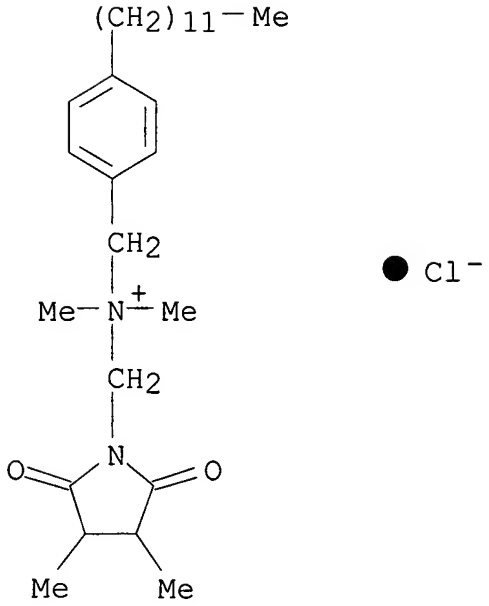
● Cl^-

RN 1433-24-5 HCA
CN 1-Pyrrolidinemethanaminium, N-[(4-dodecylphenyl)methyl]-N,N-dimethyl-2,5-dioxo-, chloride (9CI) (CA INDEX NAME)



● Cl^-

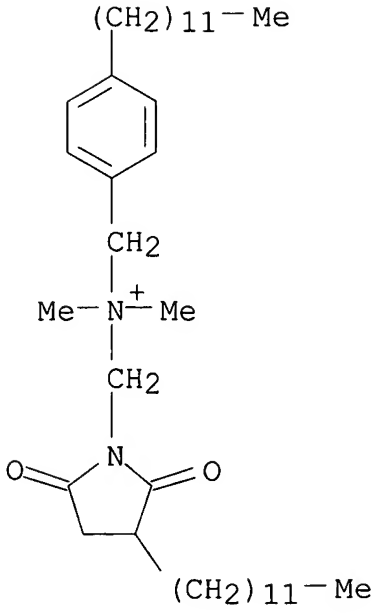
RN 1433-26-7 HCA
CN 1-Pyrrolidinemethanaminium, N-[(4-dodecylphenyl)methyl]-N,N,3,4-tetramethyl-2,5-dioxo-, chloride (9CI) (CA INDEX NAME)



RN 31426-56-9 HCA
CN 1-Pyrrolidinemethanaminium, 3-(dodecenyl)-N-[(4-dodecylphenyl)methyl]-N,N-dimethyl-2,5-dioxo-, chloride (9CI) (CA INDEX NAME)

CM 1

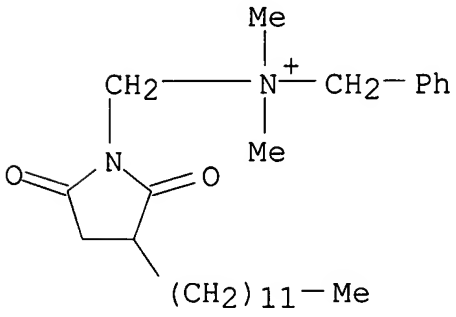
CRN 54514-84-0
CMF C38 H67 N2 O2



RN 31605-71-7 HCA
CN Ammonium, benzyl[[2-(dodecenyl)succinimido]methyl]dimethyl-, chloride (8CI) (CA INDEX NAME)

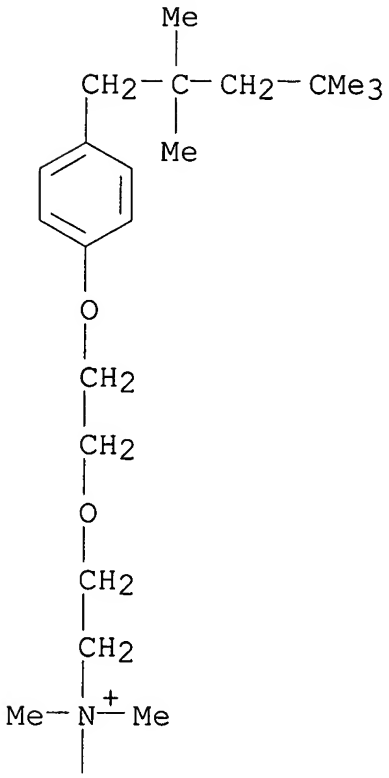
CM 1

CRN 47656-76-8
CMF C26 H43 N2 O2

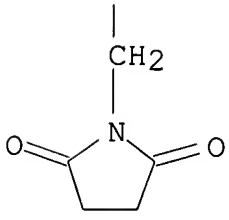


RN 106336-73-6 HCA
CN Dimethyl(succinimidomethyl)[2-[2-[p-(2,2,4,4-tetramethylpentyl)phenoxy]ethoxy]ethyl]ammonium chloride (7CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



● Cl^-

IT **1433-22-3**, Ammonium, dodecyldimethyl(succinimidomethyl), chloride **1433-24-5**, Ammonium, (p-dodecylbenzyl)dimethyl(succinimidomethyl), chloride **1433-26-7**, Ammonium, [(2,3-dimethylsuccinimido)methyl](p-

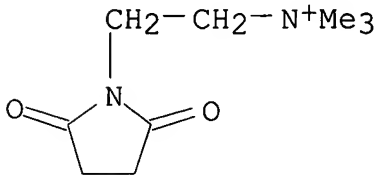
dodecylbenzyl)dimethyl, chloride **31426-56-9**, 1-Pyrrolidinemethanaminium, 3-(dodecenyl)-N-[(4-dodecylphenyl)methyl]-N,N-dimethyl-2,5-dioxo-, chloride **31605-71-7**, Ammonium, benzyl[[2-(dodecenyl)succinimido]methyl]dimethyl-, chloride **106336-73-6**, Ammonium, dimethyl(succinimidomethyl)[2-[2-[p-(2,2,4,4-tetramethylpentyl)phenoxy]ethoxy]ethyl], chloride
(prepn. of)

L34 ANSWER 30 OF 30 HCA COPYRIGHT 2006 ACS on STN
48:60147 Original Reference No. 48:10571e-i Synthesis of muscle relaxants. Hromatka, O.; Skopalik, C. (Univ. Vienna). Monatshefte fuer Chemie, 84, 919-24 (Unavailable) 1953. CODEN: MOCMB7. ISSN: 0026-9247.

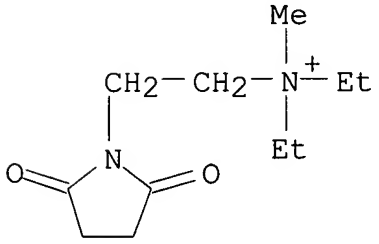
AB cf. C.A. 48, 4437h; Phillips, C.A. 47, 495b. MeO2C(CH2)nCO2Me (I, n = 6) (10.1 g.), 23.2 g. Et2NCH2CH2NH2 (II), and 15 ml. abs. EtOH heated 48 hrs. at 140-50° in a sealed tube, and the product fractionated in high vacuo, gave 77.5% Et2NCH2CH2NHCO(CH2)nCONHCH2CH2NEt2, (III) (n = 6), m. 78° (needles from abs. alc.) (1 g. is sol. in 20-25 ml. boiling ether); di-HCl salt, m. 129° (0.2 g. from 20 ml. EtOAc and 7 ml. CHCl3); picrate, m. 167° (from EtOH-MeOH-Me2CO). Similarly 5.2 g. I. (n = 8), 13.0 g. II, and 10 ml. abs. EtOH gave 80% III (n = 8), m. 81° (needles, 7.2 g., from 100 ml. ether and 10 ml. Me2CO), picrate, m. 116° (from EtOH); 1.76 g. I (n = 2), 1.8 g. Me2NCH2CH2NH2, and 10 ml. abs. EtOH gave 78% the imide (IV), b0.001 100-10° (air bath temp.); 7.3 g. I (n = 2), 23.2 g. II, and 15 ml. abs. EtOH gave 89.5% N-(β-diethylaminoethyl)succinimide (V), b12 149-50°; HCl salt, m. 210° (from abs. EtOH); picrate, m. 156° (yellow needles from abs. EtOH). III (n = 6) (1.23 g.) in 10 ml. abs. EtOH refluxed 1 hr. with 2 ml. MeI with protection from moisture, the mixt. treated with abs. ether., and cooled many days in ice gave 96% bis(methiodide), m. 134.5° (from EtOH-Me2CO); similarly III (n = 6) and EtI gave 62.5% bis(ethiodide), m. 183-3.5°; III (n = 8) and EtI gave 88% bis(ethiodide), m. 169° (from CHCl3-Me2CO-ether); IV and MeI gave 63% methiodide, m. 314-15° (decompn.) (from alc.); V and MeI gave 72% methiodide, m. 170.5° (from abs. alc.), and V and EtI gave 73% ethiodide, m. 166° (from ether-alc.). Also prepd. III (n = 0).2MeI (94% yield), m. 268-70°; III (n = 0).2EtI (85% yield), m. 279° (decompn.); III (n = 4).2MeI (91% yield), m. 139-40°; III (n = 4).2EtI (96% yield), m. 193°.

IT **73347-47-4**, Ammonium, trimethyl(2-succinimidoethyl)-, iodide **855946-78-0**, Ammonium, diethylmethyl(2-succinimidoethyl)-, iodide **857593-46-5**, Ammonium, triethyl(2-succinimidoethyl)-, iodide
(prepn. of)

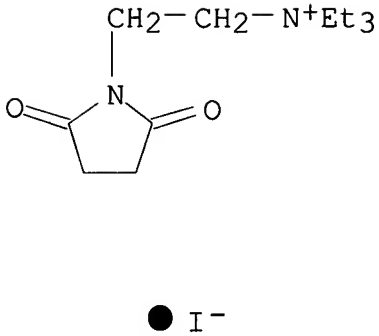
RN 73347-47-4 HCA
CN 1-Pyrrolidineethanaminium, N,N,N-trimethyl-2,5-dioxo-, iodide (9CI) (CA INDEX NAME)



RN 855946-78-0 HCA
CN Ammonium, diethylmethyl(2-succinimidoethyl)-, iodide (5CI) (CA INDEX NAME)



RN 857593-46-5 HCA
CN Ammonium, triethyl(2-succinimidoethyl)-, iodide (5CI) (CA INDEX NAME)



IT **73347-47-4**, Ammonium, trimethyl(2-succinimidoethyl)-, iodide **855946-78-0**, Ammonium, diethylmethyl(2-succinimidoethyl)-, iodide **857593-46-5**, Ammonium, triethyl(2-succinimidoethyl)-, iodide
(prepn. of)